Dictionary of Organic Compounds

FIFTH EDITION

SPRINGER-SCIENCE+BUSINESS MEDIA, B.V.

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EIGHTH SUPPLEMENT

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Treat all organic compounds as if they have dangerous properties.

The publisher makes no representation, express or implied, with regard to the accuracy of the information contained in this Dictionary, and cannot accept any legal responsibility or liability for any errors or omissions that may be made.

The specific information in this publication on the hazardous and toxic properties of certain compounds is included to alert the reader to possible dangers associated with the use of those compounds. The absence of such information should not however be taken as an indication of safety in use or misuse.

Eighth Supplement

Introduction

For detailed information about how to use DOC 5, see the Introduction in Volume 1 of the Main Work.

1. Using DOC 5 Supplements

As in the Main Work volumes, every Entry is numbered to assist ready location. The DOC Number consists of a letter of the alphabet followed by a five-digit number. In this eighth supplement the first digit is invariably 8. Cross-references within the text to Entries having numbers beginning with zero refer to Main Work Entries and with 1, 2, 3, 4, 5, 6 or 7 refer to the first seven supplements.

Where a Supplement Entry contains additional or corrected information referring to an Entry in the Main Work or earlier supplements, the whole Entry is reprinted, with the accompanying statement "Updated Entry replacing . . .". In such cases, the new Entry contains all of the information which appeared in the former Entry, except for any which has been deliberately deleted. In such cases there is therefore no necessity for the user to consult the Main Work or previous supplements.

2. Literature Coverage

In compiling this Supplement the primary literature has been surveyed to mid-1989. A considerable number of compounds from the older literature have also been included for the first time.

3. Indexes

The indexes in the Supplement cover the Sixth, Seventh and Eighth supplements. A cumulative index volume to Supplements 1–5 inclusive was issued as part of the Fifth Supplement. In order to find a compound in DOC, look first in the Eighth Supplement, then in the Fifth Supplement cumulative indexes, then in the Main Work indexes.

No CAS Registry Number Index is included in this Supplement, for reasons of pressure on space. A CAS Index was published with the Seventh Supplement, and will next reappear as part of the Tenth Supplement.

4. Symbols

The additional symbol † after a chemical name has been introduced beginning with this supplement, to denote a (trivial) name which appears in the literature more than once for different compounds (usually natural products).

5. Additional registry numbers

Some entries in DOC now carry additional Chemical Abstracts Service (CAS) registry numbers, which have been introduced to assist readers carrying out further searches (especially online searches) on substances included in DOC entries.

A small proportion of these may be duplicate numbers, but the majority are numbers which although clearly referring to the DOC entry under which they are given, cannot be unequivocally assigned to one of the substances covered by that entry, for example unfavoured tautomers and other variants for which no physical properties can be reported.

The additional numbers are given in smaller type after the text of the entry, and immediately before the references.

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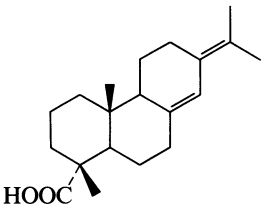
A

8(14),13(15)-Abietadien-18-oic acid — A-80001

Neoabietic acid

[471-77-2]



$C_{20}H_{30}O_2$ M 302.456

Isol. from resins of *Pinus* spp., *Abies* spp. and *Agathis microstachys*. Cryst. (EtOH aq.). Mp 173-173.5° (167-169°) (sealed tube under N_2). $[\alpha]_D^{25}$ +161.6° (c, 2.5 in 95% EtOH). Air-sensitive. Dextrosapinic acid was a mixt. of Abietic and Neoabietic acids.

Cyclohexylamine salt: Needles (EtOH aq.). Mp 211-214° dec. $[\alpha]_D^{27}$ +110.2° (c,0.295 in 95% EtOH aq.).

Harris, G.C. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 334, 339.
Schuller, W. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2563 (*isol, props, struct*)
Carman, R.M. *et al*, *Aust. J. Chem.*, 1966, **19**, 2403 (*isol*)

7,13-Abietadien-18-ol — A-80002

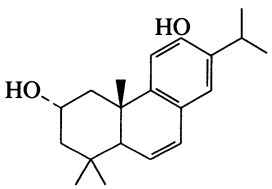
Abietinol

$C_{20}H_{32}O$ M 288.472

Isol. from *Pinus sylvestris* and *Abies sibirica*. Cryst. Mp 85.5-87°. $[\alpha]_D$ −132.5° (c, 2 in EtOH).

Erdtman, H. *et al*, *Acta Chem. Scand.*, 1963, **17**, 1826.
Chirkova, M.A. *et al*, *Khim. Prir. Soedin.*, 1966, **2**, 99.

6,8,11,13-Abietatriene-2,12-diol — A-80003



$C_{20}H_{28}O_2$ M 300.440

2α-form

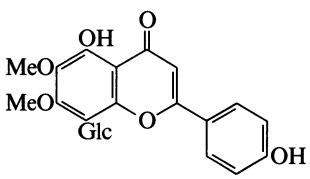
6,7-*Dehydrosalviol*

Caustic of *Salvia texana*. Yellow oil.

Gonzalez, A.G. *et al*, *J. Chem. Res.* (*S*), 1989, 132.

Abrusin — A-80004

[120727-02-8]



$C_{23}H_{24}O_{11}$ M 476.436

Constit. of *Abrus precatorius*. Cryst. Mp 270-275° dec.

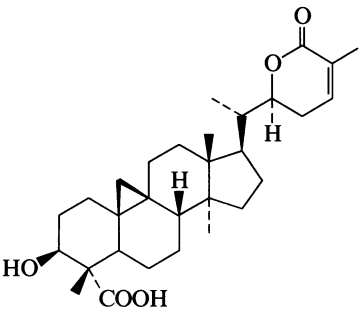
2″-O-*β-Apiofuranosyl:* [120727-04-0]. ***Abrusin 2″-O-apioside***

$C_{28}H_{32}O_{15}$ M 608.552

Constit. of *A. precatorius*. Cryst. Mp 258-263° dec. Substituted in the glucosyl residue.

Markham, K.R. *et al*, *Phytochemistry*, 1988, **27**, 299.

Abrusogenin — A-80005



$C_{30}H_{44}O_5$ M 484.675

Constit. of *Abrus precatorius*. Mp 278-280°. $[\alpha]_D$ +37° (c, 0.1 in $CHCl_3$/MeOH).

3-O-*β-D-Glucopyranoside:* ***Abrusoside* A**

$C_{36}H_{54}O_{10}$ M 646.817

Constit. of *A. precatorius*. Cryst. Mp 278-280°. $[\alpha]_D$ +11.2° (c, 0.31 in Py).

3-O-[*β-D-Glucopyranosyl-(1→2)-β-D-6-methylglucuronopyranoside*]: ***Abrusoside* B**

$C_{43}H_{64}O_{16}$ M 836.969

Constit. of *A. precatorius*. Cryst. Mp 243-245°. $[\alpha]_D$ +5.8° (c, 0.35 in Py).

3-O-[*β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside*]: ***Abrusoside* C**

$C_{42}H_{64}O_{15}$ M 808.959

Constit. of *A. precatorius*. Cryst. Mp 260-262°. $[\alpha]_D$ +31.4° (c, 0.34 in Py).

3-O-[*β-D-Glucopyranosyl-(1→2)-β-D-glucuronopyranoside*]: ***Abrusoside* D**

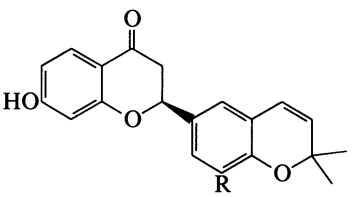
$C_{42}H_{62}O_{16}$ M 822.942

Constit. of *A. precatorius*. Cryst. Mp 237-239°. $[\alpha]_D$ +9.9° (c, 0.31 in Py).

Choi, Y.-H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1118 (*isol, pmr, cmr, cryst struct*)

Abyssinone I — A-80006

7-Hydroxy-2′,2′-dimethyl-[2,6′-bi-2H-1-benzopyran]-4(3H)one



R = H

$C_{20}H_{18}O_4$ M 322.360

(S)-form [77263-07-1]

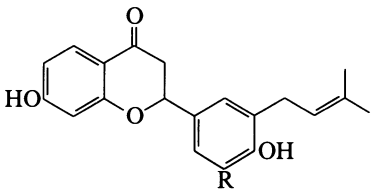
Isol. from *Erythrina abyssinica*. Shows antimicrobial activity. CA name incorrect.

Kamat, V.S. *et al*, *Heterocycles*, 1981, **15**, 1163 (*isol, uv, pmr, cd, struct, abs config*)

Abyssinone II A-80007

2,3-Dihydro-7-hydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4H-1-benzopyran-4-one,9CI. 4′,7-Dihydroxy-3′-C-prenylflavanone

[77263-08-2]



R = H

$C_{20}H_{20}O_4$ M 324.376

Isol. from *Erythrina abyssinica*. Shows antimicrobial props. Opt. inactive; CAS no. refers to the (*S*)-form.

Kamat, V.S. *et al*, *Heterocycles*, 1980, **15**, 1163 (*isol, uv, pmr, struct*)

Abyssinone III A-80008

7-Hydroxy-2,2′-dimethyl-8′-(3-methyl-2-butenyl)-[2,6′-bi-2H-1-benzopyran]-4(3H)one, 9CI

As Abyssinone I, A-80006 with

R = $-CH_2CH{=}C(CH_3)_2$

$C_{25}H_{26}O_4$ M 390.478

(S)-form [77263-09-3]

Isol. from *Erythrina abyssinica*. Shows antimicrobial activity.

Kamat, V.S. *et al*, *Heterocycles*, 1980, **15**, 1163 (*isol, uv, pmr, cd, struct, abs config*)

Abyssinone IV A-80009

2,3-Dihydro-7-hydroxy-2-[4-hydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-4H-1-benzopyran-4-one, 9CI. 4′,7-Dihydroxy-3′,5′-di-C-prenylflavanone

[77263-10-6]

As Abyssinone II, A-80007 with

R = $-CH_2CH{=}C(CH_3)_2$

$C_{25}H_{28}O_4$ M 392.494

Isol. from *Erythrina abyssinica*. Shows antimicrobial props. CAS no. refers to (*S*)-form but the isolate was opt. inactive.

5-Hydroxy: [77263-11-7]. ***Abyssinone V.*** *4′,5,7-Trihydroxy-3′,5′-di-C-prenylflavanone*

$C_{25}H_{28}O_5$ M 408.493

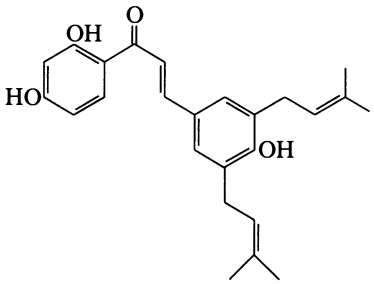
Isol. from *E. abyssinica*. Shows antimicrobial props. CAS no. refers to (S)-form but the isolate was opt. inactive.

Kamat, V.S. *et al*, *Heterocycles*, 1980, **15**, 1163 (*isol, uv, pmr, struct*)

Abyssinone VI A-80010

3-[4-Hydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-(4-hydroxyphenyl)-2-propen-1-one, 9CI. 2′,4,4′-Trihydroxy-3,5-di-C-prenylchalcone

[77263-12-8]



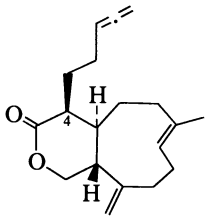
$C_{25}H_{28}O_4$ M 392.494

Isol. from *Erythrina abyssinica*. Shows antimicrobial props.

Kamat, V.S. *et al*, *Heterocycles*, 1980, **15**, 1163 (*isol, uv, pmr, struct*)

Acalycixeniolide B A-80011

Updated Entry replacing A-60011



$C_{19}H_{26}O_2$ M 286.413

Constit. of gorgonian *Acalycigorgia inermis*. Inhibits cell division in fertilised starfish eggs.

4-epimer: ***Acalycisceniolide B′***

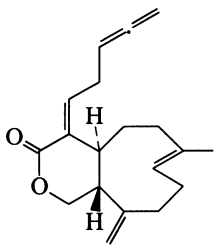
$C_{19}H_{26}O_2$ M 286.413

Constit. of *A.* sp. Oil. $[\alpha]_D$ +15° (c, 0.25 in $CHCl_3$).

Fusetani, Y. *et al*, *Tetrahedron*, 1989, **45**, 1647.

Acalycixeniolide C A-80012

[121769-80-0]



$C_{19}H_{24}O_2$ M 284.397

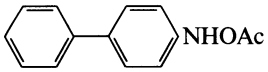
Constit. of *Acalycigorgia* sp. Cytotoxic, inhibits cell division of fertilised starfish eggs. Oil. $[\alpha]_D$ +208° (c, 0.20 in $CHCl_3$).

Fusetani, N. *et al*, *Tetrahedron*, 1989, **45**, 1647.

N-Acetoxy-4-aminobiphenyl A-80013

N-(*Acetyloxy*)-[*1,1'-biphenyl*]-*4-amine*, *9CI*. O-*Acetyl*-N-(*4-biphenylyl*)*hydroxylamine*

[119273-47-1]

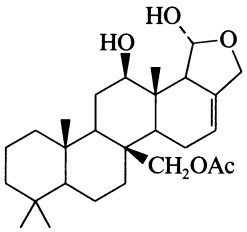


$C_{14}H_{13}NO_2$ M 227.262

Postulated proximal carcinogen of the carcinogenic 4-aminobiphenyl. Bright-yellow cryst. (Et_2O/pet. ether at −30°). Dec. in 1hr >10°.

Famulok, M. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1989, **28**, 337 (*synth*, *pmr*, *cmr*, *struct*)

24-Acetoxy-12-deacetyl-12-epideoxoscalarin A-80014



$C_{27}H_{42}O_5$ M 446.626

Constit. of *Hyatella intestinalis*. Waxy oil.

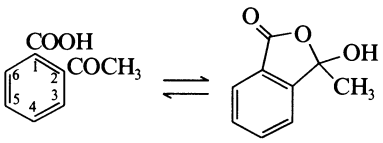
Karuso, P. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 289 (*isol*, *pmr*, *cmr*)

2-Acetylbenzoic acid, 9CI A-80015

Updated Entry replacing A-20016

3-Hydroxy-3-methylphthalide. Acetophenone-2-carboxylic acid

[577-56-0]



$C_9H_8O_3$ M 164.160

Cryst. (pet. ether). Mp 117-118°. Exists as phthalide in solid state and non-aq. soln., and as 2-acetylbenzoic acid only in aq. alkaline soln.

Me ester: [1077-79-8].
$C_{10}H_{10}O_3$ M 178.187
Liq. Bp_2 94-95°.

Nitrile: [91054-33-0]. o-*Cyanoacetophenone*
C_9H_7NO M 145.160
Mp 39-42° (48°).

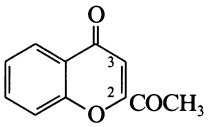
Nitrile, phenylhydrazone: Mp 205-207°.

Riemschneider, R. *et al*, *Chem. Ber.*, 1959, **92**, 1705 (*synth*)
Newman, M.S., *J. Chem. Educ.*, 1977, **54**, 191 (*synth*)
Tyman, J.H.P. *et al*, *Spectrochim. Acta*, *Part A*, 1977, **33**, 479 (*struct*, *pmr*, *cmr*, *ms*, *ir*)
Panetta, C.A. *et al*, *Synthesis*, 1977, 43 (*use*)
Durrani, A.A. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1979, 2069 (*synth*, *pmr*)
Ebert, G.W. *et al*, *J. Org. Chem.*, 1988, **53**, 4482 (*nitrile*)

2-Acetyl-4*H*-1-benzopyran-4-one, 9CI A-80016

2-Acetylchromone

[65844-02-2]



$C_{11}H_8O_3$ M 188.182

Cryst. (EtOH). Mp 137°.

Bevan, P.S. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1981, 2552 (*synth*, *ir*, *pmr*)

3-Acetyl-4*H*-1-benzopyran-4-one A-80017

3-Acetylchromone

[17422-75-2]

$C_{11}H_8O_3$ M 188.182

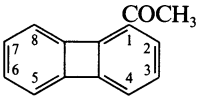
Mp 129°.

Eiden, F. *et al*, *Arch. Pharm.* (*Weinheim*, *Ger.*), 1972, **305**, 81.
Becket, G.J.P. *et al*, *Tetrahedron Lett.*, 1976, 719 (*synth*, *ir*, *pmr*)

1-Acetylbiphenylene A-80018

1-(1-Biphenylenyl)ethanone, *9CI*. *1-Biphenylenyl methyl ketone*, *8CI*

[778-92-7]



$C_{14}H_{10}O$ M 194.232

Yellow cryst. Mp 58.5°.

Martin, R.H. *et al*, *Tetrahedron*, 1964, **20**, 2373 (*pmr*)
Boulton, A.J. *et al*, *J. Chem. Soc. C*, 1968, 328 (*synth*)

2-Acetylbiphenylene A-80019

1-(2-Biphenylenyl)ethanone. 2-Biphenylenyl methyl ketone

[779-26-0]

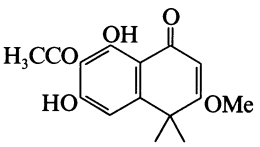
$C_{14}H_{10}O$ M 194.232

Yellow plates (MeOH). Mp 138-139°.

2,4-Dinitrophenylhydrazone: Red cryst. (AcOH). Mp 257-258°.

Baker, W. *et al*, *J. Chem. Soc.*, 1954, 1476; 1958, 2666 (*synth*, *uv*)
Droske, J.P. *et al*, *Macromolecules*, 1984, **17**, 1 (*synth*, *ir*, *pmr*)
Sutherlin, D.M. *et al*, *Macromolecules*, 1986, **19**, 257 (*synth*)

7-Acetyl-6,8-dihydroxy-3-methoxy-4,4-dimethyl-1(4*H*)-naphthalenone A-80020

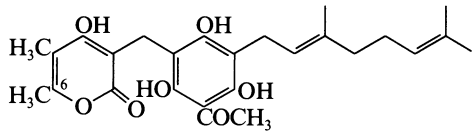


$C_{15}H_{16}O_5$ M 276.288

Pigment from root of *Cassia semicordata*. Cryst. Mp 191-192°.

Delle Monache, G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 6203.

3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-4-hydroxy-5,6-dimethyl-2*H*-pyran-2-one A-80021



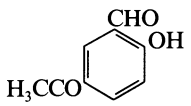
$C_{26}H_{32}O_7$ M 456.535
Constit. of *Helichrysum decumbens*. Has antifungal properties.

6-Ethyl analogue: ***3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-6-ethyl-4-hydroxy-5-methyl-2H-pyran-2-one***
$C_{27}H_{34}O_8$ M 486.561
Constit. of *H. decumbens*. Has antifungal properties.

6-Propyl analogue: ***3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-4-hydroxy-5-methyl-6-propyl-2H-pyran-2-one***
$C_{28}H_{36}O_8$ M 500.588
Constit. of *H. decumbens*. Has antifungal properties.

Tomás-Lorente, F. *et al*, *Phytochemistry*, 1989, **28**, 1613.

5-Acetyl-2-hydroxybenzaldehyde A-80022



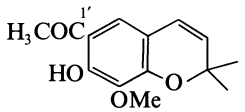
$C_9H_8O_3$ M 164.160

Me ether: 5-Acetyl-2-methoxybenzaldehyde
$C_{10}H_{10}O_3$ M 178.187
Isol. from leaves of *Encelia farinosa*. Needles (Et_2O). Mp 143-144°.

Gray, R. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 1249 (*isol, struct, synth*)

6-Acetyl-7-hydroxy-8-methoxy-2,2-dimethyl-2*H*-1-benzopyran A-80023

Updated Entry replacing A-50030
Ripariochromene A
[20770-16-5]



$C_{14}H_{16}O_4$ M 248.278
Constit. of *Eupatorium riparium*. Cryst. Mp 88.5°.

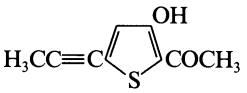
Me ether: [20819-46-9]. *6-Acetyl-7,8-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran.* ***Methylriparіochromene A***
$C_{15}H_{18}O_4$ M 262.305
Constit. of *E. riparium* and *Stevia serrata*. Low-melting solid. Mp 35°.

*Me ether, 1'-alcohol: 6-(1-Hydroxyethyl)-7,8-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran.* 6-(1-*Hydroxyethyl)eupatoriochromene* B
$C_{15}H_{20}O_4$ M 264.321
Constit. of *Ageratina riparia*. Gum. $[\alpha]_D^{24}$ −6.29° (c, 0.89 in $CHCl_3$).

Tsukayama, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 80 (*isol*)
Kohda, H. *et al*, *Phytochemistry*, 1976, **15**, 846 (*pmr*)
Banerjee, S. *et al*, *Phytochemistry*, 1985, **24**, 2681 (*isol*)
Guerin, J.-C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 171 (*isol, bibl, cryst struct*)

2-Acetyl-3-hydroxy-5-(1-propynyl)thiophene A-80024

3-Hydroxy-5-(1-propynyl)-2-thienyl methyl ketone, 8CI. 1-[3-Hydroxy-5-(1-propynyl)-2-thiophenyl]ethanone
[5556-30-9]



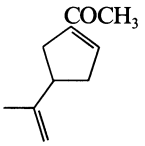
$C_9H_8O_2S$ M 180.227
Isol. from roots of *Artemisia arborescens* and *Liatris pycnostachya*. Cryst. (pet. ether). Mp 100.5° (92-94°).

Me ether: ***2-Acetyl-3-methoxy-5-(1-propynyl)thiophene***
$C_{10}H_{10}O_2S$ M 194.254
Isol. from roots of *A. arborescens*. Cryst. (pet. ether). Mp 90-91°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 2934; 1963, **96**, 584 (*isol, uv, ir, pmr, synth*)
Atkinson, R.E. *et al*, *Phytochemistry*, 1971, **10**, 454 (*isol*)

1-Acetyl-4-isopropenylcyclopentene A-80025

1-[4-(1-Methylethenyl)-1-cyclopenten-1-yl]ethanone, 9CI
[2704-76-9]



$C_{10}H_{14}O$ M 150.220
Isol. from oil of *Eucalyptus globulus*. Oil. Bp_{738} 225-225.5°, $Bp_{1.5}$ 67-68°. $n_D^{24.5}$ 1.4965.

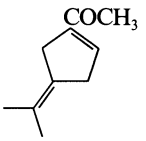
2,4-Dinitrophenylhydrazone: Red plates (EtOH). Mp 178-180°.

Semicarbazone: Cryst. (MeOH). Mp 195-196°.

Schmidt, H., *Chem. Ber.*, 1947, **80**, 528, 533 (*isol*)
Wolinsky, J. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 636 (*struct, synth*)
Conia, J.M. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 1963 (*synth, uv, ir, pmr*)
Vig, P. *et al*, *Indian J. Chem.*, 1968, **6**, 564 (*synth*)

1-Acetyl-4-isopropylidenecyclopentene A-80026

1-[4-(1-Methylethylidene)-1-cyclopenten-1-yl]ethanone, 9CI
[55873-39-7]

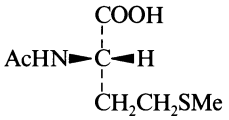


$C_{10}H_{14}O$ M 150.220
Cryst. (pentane). Mp 47-48°. Bp_8 93-94°. Descr. (1947) as a natural prod. from *Eucalyptus globulus*. This was 1-Acetyl-4-isopropenylcyclopentene, A-80025.

Bozzato, G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1974, 1005 (*synth*)
Thomas, A.F. *et al*, *Tetrahedron*, 1986, **42**, 3311 (*synth, uv, pmr, ms*)

N-Acetylmethionine, 9CI A-80027

2-(Acetylamino)-4-(methylthio)butanoic acid. Aminotylon. Methionamine. Thiomedon-Amp



(*S*)-*form*

$C_7H_{13}NO_3S$ M 191.251

(*S*)-form illustrated. Methionine therapeutic. Lipotropic agent.

(*R*)-*form* [1509-92-8]

Cryst. (EtOAc or H_2O). Mp 104-105°. $[\alpha]_D^{25}$ +20.3° (c, 4 in H_2O).

(*S*)-*form* [65-82-7]

Mp 104°. $[\alpha]_D^{25}$ −20.3°.

▷ PD0480000.

(±)-*form* [1115-47-5]

Cryst. (H_2O). Mp 114-115°.

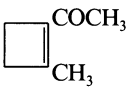
▷ PD0500000.

Wheeler, G.P. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 4604 (*synth*)
U.S. Pat., 3 028 395; *CA*, **57**, 16742 (*resoln*)
Heyns, K. *et al*, *Justus Liebigs Ann. Chem.*, 1963, **667**, 194 (*ms*)
U.K. Pat., 1 072 876; *CA*, **67**, 114015 (*resoln*)
Jung, G. *et al*, *Eur. J. Biochem.*, 1973, **35**, 436 (*cd*)
Hawkes, G.E. *et al*, *Nature (London)*, 1975, **257**, 767 (*N*-15 *nmr*)
Rotruck, J.T. *et al*, *J. Nutr.*, 1975, **105**, 331 (*metab*)
Boggs, R.W., *Adv. Exp. Med. Biol.*, 1978, **105**, 571 (*props*)
Ponnuswamy, M.N. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 917 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 571.

1-Acetyl-2-methylcyclobutene A-80028

1-(2-Methyl-1-cyclobuten-1-yl)ethanone, 9CI

[67223-99-8]



$C_7H_{10}O$ M 110.155

Liq. Bp_{16} 69-72°, Bp_6 47-48°.

Balenkova, E.S. *et al*, *Zh. Org. Khim.*, 1978, **14**, 1109; *jocet*, 1033 (*synth, ir, pmr*)
Negishi, E. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5383 (*synth, ir, pmr, cmr*)

5-Acetylthiazole A-80029

1-(5-Thiazolyl)ethanone, 9CI

[91516-28-8]

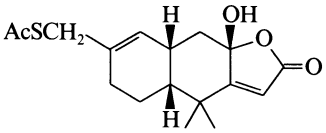
C_5H_5NOS M 127.167

Cryst. (Et_2O/hexane). Mp 68-70° (64.5-65.5°).

Kochetkov, N.K. *et al*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1959, **29**, 2294 (*synth*)
Dondoni, A. *et al*, *J. Org. Chem.*, 1988, **53**, 1748 (*synth, ir, pmr, ms*)

15-Acetylthioxyfurodysinin lactone A-80030

[122771-73-7]

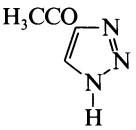


$C_{17}H_{22}O_4S$ M 322.424

Metab. of sponge *Dysidea* sp. Potent LTB_4 receptor partial agonist. Cryst. Mp 144-145°. $[\alpha]_D$ −178° ($CHCl_3$).

Carte, B. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2725.

4(5)-Acetyl-1,2,3-triazole A-80031

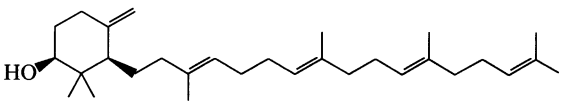


$C_4H_5N_3O$ M 111.103

Cryst. (cyclohexane). Mp 136.5°.

Banert, K., *Chem. Ber.*, 1989, **122**, 1175.

Achilleol A A-80032



$C_{30}H_{50}O$ M 426.724

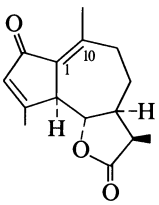
Constit. of *Achillea odorata*. $[\alpha]_D$ −10.9° (c, 0.9 in $CHCl_3$).

Barrero, A.F. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3351.

Achillin A-80033

Updated Entry replacing A-00432

[5956-04-7]



$C_{15}H_{18}O_3$ M 246.305

Constit. of *Achillea* spp. and *Artemisia* spp. Cryst. (C_6H_6/pet. ether). Mp 144-145°. $[\alpha]_D^{29}$ +160° (c, 1.2 in EtOH).

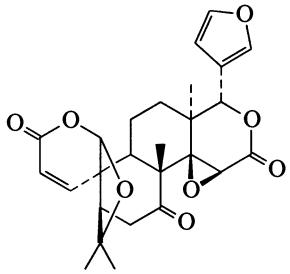
1β,10β-Epoxide: ***1β,10β-Epoxyachillin***

$C_{15}H_{18}O_4$ M 262.305

Constit. of *Artemisia lanata* and *A. assoana*. Cryst. Mp 236-238°. $[\alpha]_D$ +102° (c, 0.18 in $CHCl_3$).

Marx, J.N. *et al*, *Tetrahedron*, 1969, **25**, 2117 (*isol*)
González, A.G. *et al*, *An. Quim.*, 1976, **72C**, 695 (*isol*)
Martinéz, V. *et al*, *J. Nat. Prod. (Lloydia)*, 1988, **51**, 221 (*pmr, cmr*)
Marco, J.A. *et al*, *J. Nat. Prod. (Lloydia)*, 1989, **52**, 547 (*cryst struct, pmr, cmr*)

Acidissimin A-80034

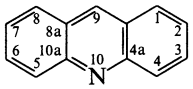


$C_{26}H_{28}O_8$ M 468.502
Constit. of *Limonia acidissima*. Cryst. Mp 284°. $[\alpha]_D$ +22° (c, 0.5 in Me_2CO).

MacLeod, J.K. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 882 (*isol, pmr, cmr*)

Acridine A-80035

Updated Entry replacing A-00457
Dibenzo[b,e]*pyridine. 9-Azaanthracene*
[260-94-6]



$C_{13}H_9N$ M 179.221
Obt. from coal tar. Parent compd. of many important dyes, alkaloids and antibacterials. Needles or prisms. Mp 111° (sealed tube)(subl. >100°). Bp ~360°. pK_a 5.60 (H_2O). Solutions show blue fluor. Five cryst. modifications known, all melting at ca. 106-111°. Triboluminescent.

▷ Toxic, irritant. LD_{50} 400 mg/kg (s.c., mice). Nasal and skin irritant. AR7175000.

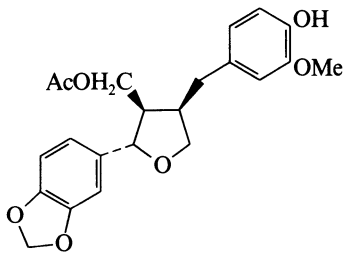
B,MeI: Red triclinic cryst.

N-*Oxide:* [10399-73-2].
$C_{13}H_9NO$ M 195.220
Yellow needles (pet. ether). Mp 169°.

Radulescu, D. *et al*, *Chem. Ber.*, 1931, **64**, 2233 (*uv*)
Corwin, A.H., *Chem. Heterocycl. Compd.*, (Elderfield, R.C. Ed.), Wiley, N.Y., 1950, **1** (*rev*)
Albert, A., *The Acridines*, Arnold, London, 1951.
Kokko, J.P. *et al*, *Spectrochim. Acta*, 1963, **19**, 1119 (*pmr*)
Nakamura, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 1135 (*cryst struct*)
Acheson, R.M., *Chem. Heterocycl. Compd.*, 2nd Ed. (Weissberger, A., Ed.), 1972, **9** (*rev, ir, uv, pmr, ms*)
Noeth, M. *et al*, *Chem. Ber.*, 1974, **107**, 3070 (*nmr*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 342.

Actifolin A-80036

[120931-63-7]

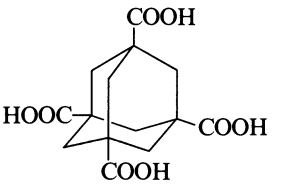


$C_{22}H_{24}O_7$ M 400.427
Constit. of *Actinodaphne longifolia*. Oil. $[\alpha]_D$ +13.3° (c, 0.48 in $CHCl_3$).

Tanaka, H. *et al*, *Phytochemistry*, 1989, **28**, 952.

1,3,5,7-Adamantanetetracarboxylic acid A-80037

Tricyclo[3.3.1.1^{3,7}]*decane-1,3,5,7-tetracarboxylic acid, 9CI*
[100884-80-8]



$C_{14}H_{16}O_8$ M 312.276
Cryst. (EtOAc). Mp 390° dec. (browns >350°).

Tetra-Me ester:
$C_{18}H_{24}O_8$ M 368.383
Cryst. (MeOH). Mp 168-169°. Bp_{12} 252°.

Tetra-Et ester:
$C_{22}H_{32}O_8$ M 424.490
56-57. Mp 56-57°.

Stetter, H. *et al*, *Chem. Ber.*, 1956, **89**, 1922 (*synth*)
Landa, S. *et al*, *Collect. Czech. Chem. Commun.*, 1959, **24**, 4004 (*synth*)
Ermer, O., *J. Am. Chem. Soc.*, 1988, **110**, 3747 (*cryst struct*)

2-Adamantanethiol A-80038

Tricyclo[3.3.1.1^{3,7}]*decane-2-thiol. 2-Mercaptoadamantane*
[23695-66-1]
$C_{10}H_{16}S$ M 168.302
Cryst. by subl. Mp 160-161°. Bp_{15} 90° subl.

Disulfide: [30979-75-0]. *Di(2-adamantyl) disulfide*
$C_{20}H_{30}S_2$ M 334.589
Cryst. (C_6H_6/MeCN). Mp 198-200°, Mp 295°.

Me thioether: [30979-72-7]. *2-(Methylthio)adamantane*
$C_{11}H_{18}S$ M 182.329
Oil. Bp_4 95-97°.

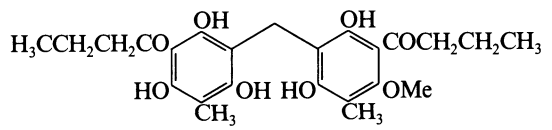
Me thioether, S-oxide: [30979-73-8]. *2-(Methylsulfinyl)adamantane*
$C_{11}H_{18}OS$ M 198.329
Shiny plates (hexane/C_6H_6). Mp 122-123°.

Me thioether, S-dioxide: [23695-67-2]. *2-(Methylsulfonyl)adamantane*
$C_{11}H_{18}O_2S$ M 214.328
Cryst. Mp 114.5-115.5°.

Greidanus, J.W. *et al*, *Can. J. Chem.*, 1969, **47**, 3715; 1970, **48**, 3593 (*synth, ir, pmr, deriv*)
Katada, T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1984, 1869 (*deriv, synth*)

Aemulin BB A-80039

1-[3-[[2,6-Dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxy-5-methylphenyl]-1-butanone, 9CI
[56226-93-8]



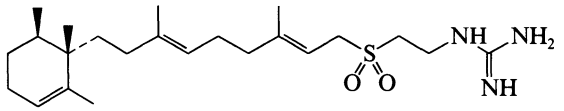
$C_{24}H_{30}O_8$ M 446.496

The BB suffix derives from the two butyryl sidechains. Other aemulins may be nat. prods. Isol. from ferns *Dryopteris aemula* and *D. pseudo-abbreviata*. Mp 90-91°.

Widén, C.-J. *et al*, *Helv. Chim. Acta*, 1975, **58**, 880 (*isol, pmr, ms, struct*)
Widén, C.-J. *et al*, *Helv. Chim. Acta*, 1976, **59**, 1725 (*occur*)

Agelasidine C A-80040

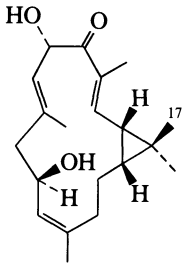
[92664-78-3]



$C_{23}H_{41}N_3O_2S$ M 423.662
Constit. of sponge *Agelas* sp.

Nakamura, H. *et al*, *J. Org. Chem.*, 1985, **50**, 2494 (*isol*)
Asao, K. *et al*, *Chem. Lett.*, 1989, 1813 (*synth*)

Agrostistachin A-80041

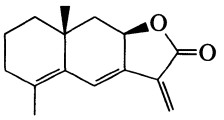


$C_{20}H_{30}O_3$ M 318.455
Constit. of *Agrostistachys hookeri*. Cryst. (EtOAc). Mp 155-157°. $[\alpha]_D$ +248° (c, 0.18 in $CHCl_3$).

17-Hydroxy: ***Hydroxyagrostistachin***
$C_{20}H_{30}O_4$ M 334.455
Constit. of *A. hookeri*. Resin. $[\alpha]_D$ +167° (c, 0.09 in $CHCl_3$).

Choi, Y.-H. *et al*, *Tetrahedron Lett.*, 1986, **27**, 5795 (*isol, cryst struct*)
Choi, Y.-H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 110 (*deriv*)

Alantodiene A-80042

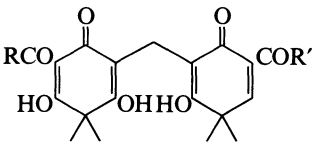


$C_{15}H_{18}O_2$ M 230.306
Constit. of *Inula racemosa*. Oil.

Kalsi, P.S. *et al*, *Phytochemistry*, 1989, **28**, 2093 (*isol, pmr*)

Albaspidins A-80043

Updated Entry replacing A-00708



Albaspidins AA, R = R′ = CH_3
AP, R = CH_3, R′ = CH_2CH_3
AB, R = CH_3, R′ = $CH_2CH_2CH_3$
PP, R = R′ = CH_2CH_3
PB, R = CH_2CH_3, R′ = $CH_2CH_2CH_3$
BB, R = R′ = $CH_2CH_2CH_3$

The suffix letters denote the side-chains (A = acetyl, P = propionyl, B = butyryl). Constits. of *Dryopteris* and *Aspidium* spp. ferns. Albaspidin 1 was a mixt. of BB, PB and PP. Albaspidin 2 was a mixt. of AB and AP. The various albaspidins disproportionate under mildly alkaline conds.

Albaspidin AA [3570-40-9]
2,2′-*Methylenebis*[6-*acetyl*-3,5-*dihydroxy*-4,4-*dimethyl*-2,5-*cyclohexadien*-1-*one*], *9CI. Albaspidin* 3
$C_{21}H_{24}O_8$ M 404.416
Cryst. (Me_2CO). Mp 170-171°.

Albaspidin AP [59092-91-0]
$C_{22}H_{26}O_8$ M 418.443

Albaspidin AB [3570-35-2]
$C_{23}H_{28}O_8$ M 432.469

Albaspidin PP [3570-39-6]
$C_{23}H_{28}O_8$ M 432.469
Mp 135-137°.

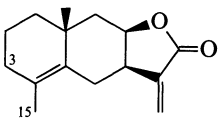
Albaspidin PB [3772-65-4]
$C_{24}H_{30}O_8$ M 446.496

Albaspidin BB [644-61-1]
Polystichalbin. White polystichum acid
$C_{25}H_{32}O_8$ M 460.523
Needles (AcOH). Mp 147-145°.

Penttila, A. *et al*, *Acta Chem. Scand.*, 1964, **18**, 344 (*isol, struct, synth*)
Launasmaa, M. *et al*, *Acta Chem. Scand.*, 1972, **26**, 89 (*synth, ms*)
Widen, C.J. *et al*, *Helv. Chim. Acta*, 1975, **58**, 880 (*isol, struct*)
Puri, H.S. *et al*, *Phytochemistry*, 1976, **15**, 343 (*isol*)
Jayasuriya, H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 325 (*isol*)

Alloalantolactone A-80044

[64340-41-6]



$C_{15}H_{20}O_2$ M 232.322
Constit. of *Inula helenium*. Oil. $[\alpha]_D$ +35.2° (c, 0.5 in $CHCl_3$).

3α,15-Dihydroxy: [119285-38-0]. ***3α,15-Dihydroxyalloalantolactone***
$C_{15}H_{20}O_4$ M 264.321
Constit. of *Ambrosia artemisioides*. Oil.

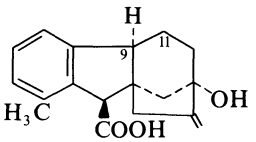
15-Acetoxy, 3α-hydroperoxy: [119285-37-9]. ***15-Acetoxy-3α-hydroperoxyalloalantolactone***
$C_{17}H_{22}O_6$ M 322.357
Constit. of *A. artemisioides*. Oil.

15-Hydroxy, 3-oxo: [119285-39-1]. ***15-Hydroxy-3-oxoalloalantolactone***
$C_{15}H_{18}O_4$ M 262.305
Constit. of *A. artemisioides*. Oil.

Ananthasubramanian, L. *et al*, *Indian J. Chem., Sect. B*, 1978, **16**, 191 (*synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1978, **17**, 1165 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551 (*deriv*)

Allogibberic acid A-80045

Updated Entry replacing A-00787
Gibberellin B
[427-79-2]



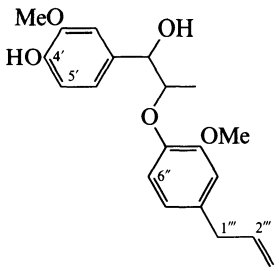
$C_{18}H_{20}O_3$ M 284.354
Isol. from *Gibberella fujikuroi* and *Lemna perpusilla*. Inhibitor of flowering. Cryst. Mp 201-203° (anhyd.). $[\alpha]_D^{20}$ −84° (EtOH).

Me ester: Mp 98-99°. $[\alpha]_D^{22}$ −82° (EtOH).

9,11-Didehydro: ***Dehydroallogibberic acid***
$C_{18}H_{18}O_3$ M 282.338
Isol. from cultures of *Gibberella fujikuroi*. Needles (Me_2CO/pet. ether). Mp 211-214° dec. $[\alpha]_D^{27}$ −37° (c, 0.2 in EtOH).

Cross, B.E., *J. Chem. Soc.*, 1954, 4670 (*isol*)
Mulholland, T.P.C. *et al*, *J. Chem. Soc.*, 1958, 2693; 1960, 3007 (*isol*)
Stork, G. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 3168 (*stereochem*)
Cross, B.E. *et al*, *J. Chem. Soc.*, 1963, 2937 (*Dehydroallogibberic acid*)
Pryce, R.J., *Phytochemistry*, 1973, **12**, 1745 (*isol*)
Voigt, D. *et al*, *Org. Mass Spectrom.*, 1978, **13**, 599 (*ms*)

2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol A-80046



$C_{20}H_{24}O_5$ M 344.407
Constit. of Oil of *Myristica fragrans*. Oil.

5'-Methoxy,Δ1'''-isomer(E-)*: 1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[2-methoxy-4-(1-propenyl)phenoxy]-1-propanol*
$C_{21}H_{26}O_6$ M 374.433
Constit. of *M. fragrans* oil. Oil.

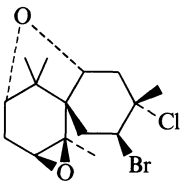
5',6''-Dimethoxy: 2-(4-Allyl-2.6-dimethoxyphenoxy)-1-(4-hydroxy-3,5-dimethoxyphenyl)-1-propanol
$C_{22}H_{20}O_7$ M 396.396
Constit. of oil of *M. fragrans*. Oil.

O4'-Me, 5'-hydroxy,6''-methoxy: 2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3-hydroxy-4,5-dimethoxyphenyl)-1-propanol
$C_{22}H_{28}O_7$ M 404.459
Constit.of oil of *M. fragrans*. Oil.

Haltori, M. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 668.

Almadioxide A-80047

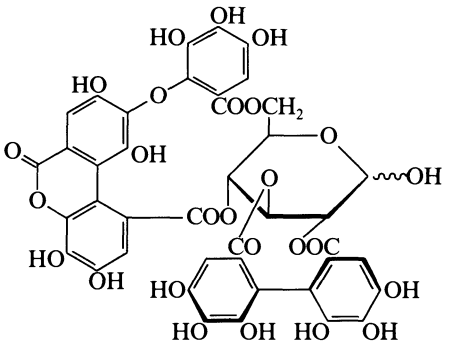
[119400-88-3]



$C_{15}H_{22}BrClO_2$ M 349.694
Constit. of alga *Laurencia intricata*. Cryst. (CH_2Cl_2/hexane). Mp 206°. $[\alpha]_D$ +4° (c, 0.7 in $CHCl_3$).

Aknin, M. *et al*, *Tetrahedron Lett.*, 1989, **30**, 559 (*cryst struct*)

Alnusiin A-80048

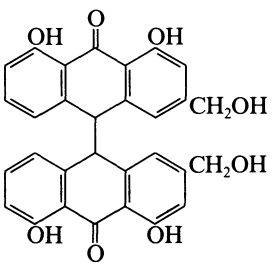


$C_{41}H_{26}O_{26}$ M 934.641
Constit. of *Alnus sieboldiana*. Amorph.

Yoshida, T. *et al*, *Heterocycles*, 1981, **16**, 1085; 1989, **29**, 861 (*isol, struct, cmr*)

Aloeemodin dianthrone A-80049

4,4',5,5'-Tetrahydroxy-2,2'-bis(hydroxymethyl)-[9,9'-bianthracene]-10,10'(9H,9'H)-dione, 9CI. Aloeemodin bianthrone
[4461-75-0]



$C_{30}H_{22}O_8$ M 510.499
Isol. from leaves of *Cassia angustifolia* and fruits of *Frangula alnus*. Dark-brown solid. Mp >260° dec. λ_{max} 220, 270 nm.

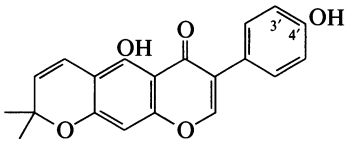
Auterhoff, H. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1960, **293**, 918 (*synth, ir, uv*)
Lemli, J. *et al*, *Pharm. Weekbl.*, 1964, **99**, 589 (*isol*)
Lemli, J., *J. Nat. Prod.* (*Lloydia*), 1965, **28**, 63 (*isol*)

Alpinumisoflavone A-80050

Updated Entry replacing A-00851

*5-Hydroxy-7-(4-hydroxyphenyl)-2,2-dimethyl-2*H,*6*H-*benzo[1,2-*b*:5,4-*b′*]dipyran-6-one, 9CI. 5-Hydroxyerythrinin* A

[34086-50-5]



$C_{20}H_{16}O_5$ M 336.343

Constit. of the twigs of *Laburnum alpinum* and of the bark of *Erythrina variegata*. Also from *Calopogonium mucunoides* and *Millettia thonningii*. Cryst. (Me_2CO/hexane or $CHCl_3$/EtOAc). Mp 213-214°.

Di-Ac: Cryst. (MeOH or EtOAc/pet. ether). Mp 135-137° (219°).

4′-Me ether: [27762-87-4].
$C_{21}H_{18}O_5$ M 350.370
Isol. from seeds of *C. mucunoides*.

Di-Me ether: [34086-56-1].
$C_{22}H_{20}O_5$ M 364.397
Isol. from seeds of *Derris robusta*. Cryst. (C_6H_6). Mp 119-120°.

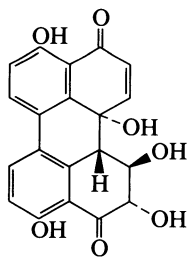
4′-Me ether, 3′-hydroxy: ***3′-Hydroxyalpinumisoflavone 4′-methyl ether***
$C_{21}H_{18}O_6$ M 366.370
Isol. from seeds of *M. thonningii*.

Jackson, B. *et al*, *J. Chem. Soc. C*, 1971, 3389 (*isol, struct*)
Jain, A.C. *et al*, *J. Org. Chem.*, 1974, **39**, 2215 (*synth*)
Vilain, C. *et al*, *Bull. Soc. R. Sci. Liege*, 1975, **44**, 306; *CA*, **84**, 74136e (4′-*O*-Methylalpinumisoflavone)
Deshpande, V.H. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 205 (*isol*)
Chibber, S.S. *et al*, *Indian J. Chem., Sect. B*, 1979, **18**, 471 (*isol, deriv*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev*)

Alterlosin I A-80051

*5,6,6*a,*6*b-*Tetrahydro-3,5,6,6*b,*10-pentahydroxy-4,9-perylenedione, 9CI*

[120462-02-4]



$C_{20}H_{14}O_7$ M 366.326

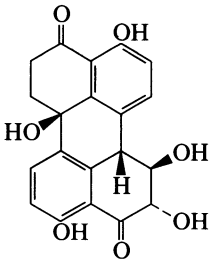
Metab. of *Alternaria alternata*. Phytotoxin. Cryst. Mp 191-193°. $[\alpha]_D$ +122° (c, 0.21 in MeOH).

Stierle, A.C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 42 (*isol, ir, pmr*)

Alterlosin II A-80052

*1,2,6*b,*7,8,12*b-*Hexahydro-4,7,8,10,12*b-*pentahydroxy-3,9-perylenedione, 9CI*

[120462-03-5]



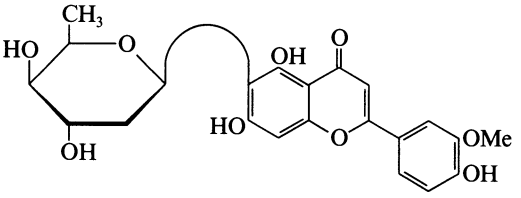
$C_{20}H_{16}O_7$ M 368.342

Metab of *Alternaria alternata*. Phytotoxin. Cryst. Mp 185-187°. $[\alpha]_D$ +131° (c, 0.2 in MeOH).

Stierle, A.C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 42 (*isol, ir, pmr*)

Alternanthin A-80053

[119269-48-6]



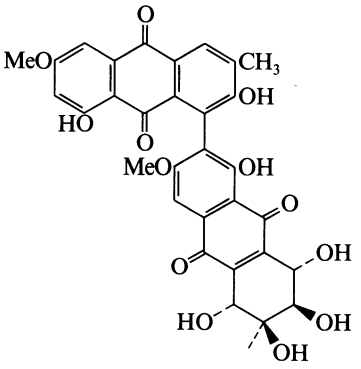
$C_{22}H_{22}O_9$ M 430.410

Constit. of *Alternanthera philoxeroides*. Yellow needles (MeOH). Mp 225-227°. $[\alpha]_D$ +86.2° (c, 0.23 in MeOH).

Zhou, B.-N. *et al*, *Phytochemistry*, 1988, **27**, 3633.

Alterporriol C A-80054

[118074-08-1]



$C_{32}H_{26}O_{13}$ M 618.550

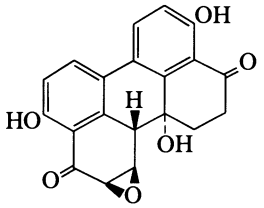
Metab. of *Alternaria porri*. Dark-red amorph. solid. Mp >300° dec. $[\alpha]_D^{25}$ −268° (c, 0.05 in EtOH).

Suemitsu, R. *et al*, *Phytochemistry*, 1988, **27**, 3251.

Altertoxin II A-80055

Stemphyltoxin II

[56257-59-1]



$C_{20}H_{14}O_6$ M 350.327

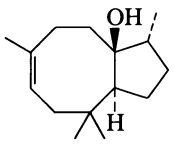
Isol. from *Alternaria tenuis* and *A. mali* and *Stemphylium botryosum*. Phototoxin. Active against gram-positive bacteria. Orange cryst. solid. Mp 245-250° (300° dec.). $[\alpha]_D$ +636° (c, 0.001 in $CHCl_3$).

▷ BC9625300.

Pero, R.W. *et al*, *EHP Environ. Health Perspect.*, 1973, **4**, 87 (*isol*)
Harvan, D. *et al*, *Adv. Chem. Ser.*, 1976, **149**, 344 (*rev*)
Griffin, G.F. *et al*, *J. Chromatogr.*, 1983, **280**, 363 (*isol, hplc*)
Arnone, A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1986, 525 (*Stemphyltoxins*)
Stack, M.E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1986, **49**, 866 (*pmr, cmr, struct*)
Cole, R.J. *et al*, *Handbook of Toxic Fungal Metabolites*, Academic Press , N.Y., 1981, 640.

4-Ambiguen-1-ol A-80056

1-Hydroxy-4-ambiguene



$C_{15}H_{26}O$ M 222.370

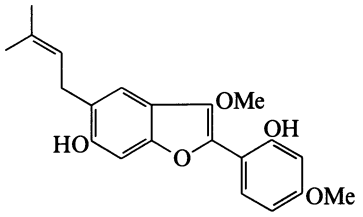
Constit. of *Helichrysum bilobum* ssp. *bilobum*. Oil. $[\alpha]_D^{24}$ −45° (c, 0.89 in $CHCl_3$).

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 543.

Ambofuranol A-80057

2-(2-Hydroxy-4-methoxyphenyl)-3-methoxy-5-(3-methyl-2-butenyl)-6-benzofuranol, 9CI. 6-Hydroxy-2-(2-hydroxy-4-methoxyphenyl)-3-methoxy-5-C-prenylbenzofuran

[76869-00-6]



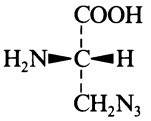
$C_{21}H_{22}O_5$ M 354.402

Isol. from bulb bark of *Neorautanenia amboensis*. Needles (C_6H_6 or EtOH). Mp 147-148°.

Breytenbach, J.C. *et al*, *Tetrahedron Lett.*, 1980, 4535 (*isol, pmr, ms, struct*)

2-Amino-3-azidopropanoic acid A-80058

3-Azidoalanine



(*S*)-*form*

$C_3H_6N_4O_2$ M 130.106

(S)-form [105661-40-3]

L-form

Metabolite isol. from *Salmonella* grown in the presence of azide. Cryst. (H_2O/MeOH/Me_2CO at −20°). Mp 174-175° dec.

▷ Mutagenic.

Arnold, L.D. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2237 (*synth, ir, pmr, cmr, ms*)

4-Aminobenzimidazole A-80059

Updated Entry replacing A-01018

1H-Benzimidazol-4-amine, 9CI

[4331-29-7]

$C_7H_7N_3$ M 133.152

Prisms ($CHCl_3$). Mp 120-121°.

▷ DD5780000.

B,2HCl: [37724-28-0].
Cryst. (MeOH). Mp 247-249° dec.

1-Oxide:
$C_7H_7N_3O$ M 149.152
Cryst. + $1H_2O$ (H_2O). Mp 118-120°.

1-Oxide; B-2HCl: Cryst. (conc. HCl). Mp 224-226°.

3-Oxide:
$C_7H_7N_3O$ M 149.152
Cryst. + $1H_2O$ (H_2O). Mp 108-110°.

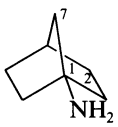
3-Oxide; B,2HCl: Cryst. (conc. HCl). Mp 190-192° dec.

Van der Want, G.M., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1948, **67**, 45 (*synth*)
Fisher, E.C. *et al*, *J. Org. Chem.*, 1958, **23**, 1944 (*synth*)
Keiser, S. *et al*, *Pharmazie*, 1972, **27**, 287 (*rev*)
Harvey, I.W. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1939 (*oxides*)

1-Aminobicyclo[2.2.1]heptane A-80060

Bicyclo[2.2.1]heptan-1-amine, 9CI. 1-Aminonorbornane

[21245-51-2]



$C_7H_{13}N$ M 111.186

Liq. Bp 142-145°. pK_a 10.20.

B,HCl: [75934-56-4].
Solid. Mp >350°.

Picrate: Cryst. (EtOAc/pet. ether). Mp 210°.

[107474-88-4, 107474-89-5]

Werner, R.B. *et al*, *J. Med. Chem.*, 1961, **4**, 183 (*synth*)
Wiberg, K.B. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 3188.
Deutsch, J. *et al*, *Isr. J. Chem.*, 1972, **10**, 51 (*ms*)
Golzke, V. *et al*, *Nouv. J. Chim.*, 1978, **2**, 169; *CA*, **89**, 42069x (*synth*)
Pachter, R. *et al*, *Theochem*, 1986, **30**, 143; *CA*, **105**, 60240z (*cmr*)
Della, E.W. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 2746 (*synth, N-15 nmr*)

7-Aminobicyclo[2.2.1]heptane A-80061

Bicyclo[2.2.1]heptan-7-amine, 9CI. 7-Aminonorbornane

[35092-58-1]

$C_7H_{13}N$ M 111.186

Oily solid or liq. Bp 147-152°, Bp_8 66-67.5°.

B,HCl: [35092-59-2].
Cryst.

N-*Methoxycarbonyl:*
$C_9H_{15}NO_2$ M 169.223
Long needles. Mp 68-69°.

N-*Ac:*
$C_9H_{15}NO$ M 153.224
Cryst. (hexane). Mp 130-131°.

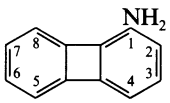
N-*Chloroacetyl:*
$C_9H_{14}ClNO$ M 187.668
Cryst. (pet. ether). Mp 84-85° (80°).

Boehme, W.R. *et al, J. Med. Chem.*, 1961, **4**, 183 (*synth*)
Zalkow, L.H. *et al, J. Org. Chem.*, 1963, **28**, 3303 (*synth, ir, pmr, derivs*)
Stille, J.K. *et al, J. Am. Chem. Soc.*, 1972, **94**, 8489 (*deriv*)
Hermes, M.E. *et al, J. Org. Chem.*, 1972, **37**, 2969 (*synth, pmr*)
Pachter, R. *et al, Theochem*, 1986, **30**, 143; *CA*, **105**, 60240z (*cmr*)
Fukunage, K. *et al, Synthesis*, 1987, 1097 (*synth*)

1-Aminobiphenylene A-80062

1-Biphenylenamine, 9CI

[16294-10-3]



$C_{12}H_9N$ M 167.210

Pale yellow needles (pet. ether). Mp 80-81°.

N-Ac: [16294-11-4].
$C_{14}H_{11}NO$ M 209.247
Pale yellow needles (C_6H_6). Mp 193-194°.

Barton, J.W. *et al, J. Chem. Soc. C*, 1967, 2097 (*synth, uv, pmr*)

2-Aminobiphenylene A-80063

2-Biphenylenamine

[55716-75-1]

$C_{12}H_9N$ M 167.210

Polymer intermediate. Yellow needles. Mp 123-124°.

N-Ac:
$C_{14}H_{11}NO$ M 209.247
Pale yellow plates (EtOH aq.). Mp 146-147°.

Baker, W. *et al, J. Chem. Soc.*, 1954, 1476; 1958, 2666 (*synth, deriv, uv*)
Barton, J.W. *et al, J. Chem. Soc. C*, 1967, 2097 (*pmr*)
Droske, J.P. *et al, Macromolecules*, 1984, **17**, 10.
Takeichi, T. *et al, Macromolecules*, 1986, **19**, 2093, 2103, 2108 (*use*)

4-Aminobutanal, 9CI A-80064

Updated Entry replacing A-01166

4-Aminobutyraldehyde

[4390-05-0]

$H_2NCH_2CH_2CH_2CHO$

C_4H_9NO M 87.121

2,4-Dinitrophenylhydrazone; B,HCl: Solid (EtOH). Mp 198-199°.

Di-Me acetal: [19060-15-2]. *4,4-Dimethoxybutylamine*
$C_6H_{15}NO_2$ M 133.190
Oil. Bp_{22} 83-85°.

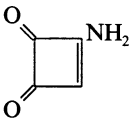
Di-Et acetal: [6346-09-4]. *4,4-Diethoxybutylamine*
$C_8H_{19}NO_2$ M 161.244
Bp 196°, $Bp_{0.5}$ 84-85°.

Burckhalter, J.H. *et al, J. Org. Chem.*, 1958, **23**, 1278 (*synth*)
Leonard, N.J. *et al, Tetrahedron Lett.*, 1960, 44 (*synth*)
Gribble, G.W. *et al, J. Org. Chem.*, 1988, **53**, 3164 (*acetal, synth, ir, pmr*)

3-Amino-3-cyclobutene-1,2-dione, 9CI A-80065

Semisquaric amide

[65842-67-3]

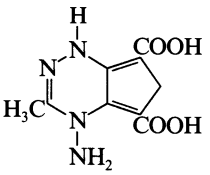


$C_4H_3NO_2$ M 97.073

Cryst. (EtOH). Mp 170° dec. An earlier report of this compd. (mp. 85° dec.) was erroneous.

Schmidt, A.H. *et al, Synthesis*, 1987, 134 (*synth, ir, pmr, cmr*)

4-Amino-4,6-dihydro-3-methyl-1*H*-cyclopenta[*e*]1,2,4-triazine-5,7-dicarboxylic acid A-80066



$C_9H_{10}N_4O_4$ M 238.202

Di-Me ester: [95927-46-1].
$C_{11}H_{14}N_4O_4$ M 266.256
Reagent for conversion of aldehydes to nitriles in good yield, *via* hydrazone formn. Mp 198-199° dec.

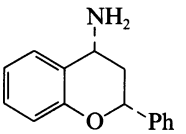
Di-Et ester: [117227-44-8].
$C_{13}H_{18}N_4O_4$ M 294.310
Reagent for conversion of aldehydes to nitriles. Mp 185-186° dec.

Neunhoeffer, H. *et al, Justus Liebigs Ann. Chem.*, 1989, 105 (*synth, ir, pmr, use*)

4-Amino-3,4-dihydro-2-phenyl-2*H*-1-benzopyran A-80067

3,4-Dihydro-2H-1-benzopyran-4-amine, 9CI. 4-Aminoflavan

[6517-15-3]



(2*R*,4*R*)-*form*

$C_{15}H_{15}NO$ M 225.290

(2R,4R)-form
(+)-cis-*form*
Mp 112° dec. $[\alpha]_D$ +14° (EtOH).

B,HCl: [29834-28-4].
Mp 281-283°. $[\alpha]_D$ +26.8° (EtOH).

N-*Ac:*
$C_{17}H_{17}NO_2$ M 267.327

Mp 208-209°. $[\alpha]_D$ +32.1°.

(2S,4S)-form

(−)-cis-*form*

Mp 112° dec. $[\alpha]_D$ −13.8° (EtOH).

B,HCl: [29834-29-5].

Mp 285-286°. $[\alpha]_D$ −26.5° (EtOH).

N-*Ac:* Mp 224-225°. $[\alpha]_D$ −14.5° (EtOH).

(2R,4S)-form

(−)-trans-*form*

Mp 116° dec. $[\alpha]_D^{20}$ −14° (c, 0.5 in EtOH).

B,HCl: Mp 263-264°. $[\alpha]_D^{20}$ −22° (c, 0.5 in EtOH).

(2S,4R)-form

(+)-trans-*form*

Mp 116°. $[\alpha]_D^{20}$ +14° (c, 0.5 in EtOH).

B,HCl: Mp 260°. $[\alpha]_D^{20}$ +24° (c, 0.5 in EtOH).

(2RS,4RS)-form

(±)-cis-*form*

B,HCl: Mp 267-270°.

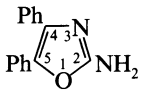
N-*Ac:* Mp 202°.

Tökés, A.L. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 89 (*resoln, abs config, bibl*)

2-Amino-4,5-diphenyloxazole A-80068

4,5-Diphenyl-2-oxazolamine, 9CI

[33119-63-0]



$C_{15}H_{12}N_2O$ M 236.273

Cryst. (pet. ether). Mp 142°.

Picrate: Mp 222°.

Gompper, R. *et al*, *Chem. Ber.*, 1959, **92**, 1944.

4-Amino-2,5-diphenyloxazole A-80069

2,5-Diphenyl-4-oxazolamine, 9CI

[121019-48-5]

$C_{15}H_{12}N_2O$ M 236.273

Plates (EtOH). Mp 261-262°. First known simple 4-aminooxazole. Various ring-substd. analogues also prepd.

Lakhan, R. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1413.

5-Amino-2,4-diphenyloxazole A-80070

2,4-Diphenyl-5-oxazolamine, 9CI

[17960-26-8]

$C_{15}H_{12}N_2O$ M 236.273

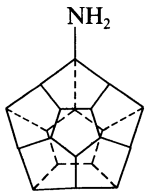
Cryst. (CH_2Cl_2). Mp 133-135°.

Poupaert, J. *et al*, *Synthesis*, 1972, 622.

Aminododecahedrane A-80071

*Tetradecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenedipentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalen-1(2*H*)-amine, 9CI. Dodecahedranamine*

[116635-07-5]



$C_{20}H_{21}N$ M 275.393

B,HCl: [116663-41-3].

Solid. Mp >250°.

N-*Ac:* [112896-39-6].

$C_{22}H_{23}NO$ M 317.430

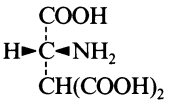
Solid. Mp >250°.

Weber, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5315 (*synth, pmr, cmr*)

2-Amino-1,1,2-ethanetricarboxylic acid, 9CI A-80072

β-Carboxyaspartic acid. Asa

[75898-26-9]



(*R*)-*form*

$C_5H_7NO_6$ M 177.113

Obt. only in racemic form from natural systems.

(R)-form [99265-42-6]

D-*form*

Synthetic.

B,HCl: [111934-05-5].

Solid. $[\alpha]_D^{25}$ −13.25° (c, 0.8 in H_2O).

N-*Ac, Tri-Me ester:* [99265-41-5].

$C_{10}H_{15}NO_7$ M 261.231

$[\alpha]_D^{20}$ +86.9° (c, 2.0 in MeOH).

*1,1-Di-*tert*-butyl ester, 2-Me ester:* [99166-13-9].

Mp 63-64°. $[\alpha]_D^{25}$ +0.4° (c, 1.0 in MeOH).

(±)-form [78000-84-7]

Isol. from the ribosomal proteins of *E. coli* and human atherosclerotic plaque. pK_a *ca* 0.8. V. sensitive to decarboxylation so difficult to detect in natural systems.

B,HCl: [78000-85-8].

Unstable.

N-Ac,Tri-Me ester: [78000-86-9].

Cryst. Mp 77-78°.

[90365-27-8]

Christy, M.R. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 3935 (*isol, synth, pmr, cmr*)

Henson, E.B. *et al*, *Tetrahedron*, 1981, **37**, 2561 (*synth, ms*)

Richey, B. *et al*, *Biochemistry*, 1982, **21**, 4819 (*cryst struct*)

Koch, T.H. *et al*, *Methods Enzymol.*, 1984, **107**, 563 (*synth, ir, pmr, cmr*)

Van Buskirk, J.J. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1984, **81**, 722 (*biochem*)

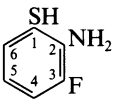
Schöllkopf, U. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 1066 (*synth*)

Williams, R.M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 482 (*synth, pmr*)

2-Amino-3-fluorobenzenethiol, 9CI A-80073

2-Fluoro-6-mercaptoaniline

[73628-29-2]



C_6H_6FNS M 143.184

Mp 92°.

Gupta, R.R. *et al*, *Synth. Commun.*, 1987, **17**, 229.

2-Amino-5-fluorobenzenethiol, 9CI **A-80074**

4-Fluoro-2-mercaptoaniline

[33264-82-3]

C_6H_6FNS M 143.184

Fine yellow cryst. (EtOH). Mp 82°.

Mital, R. *et al*, *Monatsh. Chem.*, 1971, **102**, 760 (*synth*)
Sawhney, S.N. *et al*, *J. Org. Chem.*, 1979, **44**, 1136 (*cmr*)
Gupta, R.R. *et al*, *J. Fluorine Chem.*, 1985, **28**, 381 (*synth*)

2-Amino-6-fluorobenzenethiol, 9CI **A-80075**

3-Fluoro-2-mercaptoaniline

[100493-32-1]

C_6H_6FNS M 143.184

Eur. Pat., 158 340, (1985); *CA*, **105**, 6526j.

4-Amino-2-fluorobenzenethiol, 8CI **A-80076**

3-Fluoro-4-mercaptoaniline

[15178-52-6]

C_6H_6FNS M 143.184

Pohloudek-Fabini, R. *et al*, *CA*, 1967, **67**, 73287s (*synth*)

4-Amino-3-fluorobenzenethiol, 9CI **A-80077**

2-Fluoro-4-mercaptoaniline

[15178-48-0]

C_6H_6FNS M 143.184

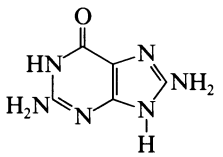
[100280-13-5]

Pohlondek-Fabini, R. *et al*, *CA*, 1967, **67**, 73287s.

8-Aminoguanine **A-80078**

*2,8-Diamino-1,7-dihydro-6*H*-purin-6-one, 9CI. 2,8-Diaminohypoxanthine. 2,8-Diamino-6-hydroxypurine*

[28128-41-8]

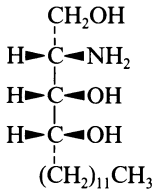


$C_5H_6N_6O$ M 166.142

Solid. Mp >240°.

Holmes, R.E. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 1772 (*synth*)
Lin, T.S. *et al*, *J. Med. Chem.*, 1985, **28**, 1194 (*synth*)

2-Amino-1,3,4-hexadecanetriol **A-80079**



$C_{16}H_{35}NO_3$ M 289.457

(2S,3S,4R)-form

Common phytosphingosine, occurring for example in Acanthocerebrosides.

O,N,N,N-*Tetra-Ac:* [114379-45-2].
$C_{24}H_{43}NO_7$ M 457.606

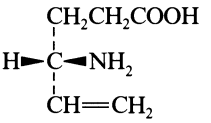
Viscous liq. $[\alpha]_D^{25}$ +27.9° (c, 1.5 in $CHCl_3$).

Sugiyama, S. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 619 (*abs config, bibl*)

4-Amino-5-hexenoic acid, 9CI **A-80080**

***Vigabatrin*, BAN, INN.** *γ-Vinyl GABA. GVG. MDL 71754. RMI 71754*

[60643-86-9]



(*S*)-*form*

$C_6H_{11}NO_2$ M 129.158

(S)-form [74046-07-4]

Pharmacol active isomer. Anticonvulsant. Inhibitor of GABA transaminase. Cryst. (EtOH/2-propanol). $[\alpha]_D$ +12.4° (c, 0.5 in H_2O).

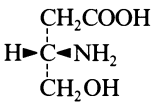
(±)-form [68506-86-5]

Cryst. (EtOH aq.).

[77162-51-7]

U.S. Pat., 3 960 927; *CA*, **85**, 143512 (*synth*)
Palfreyman, M.G. *et al*, *Biochem. Pharmacol.*, 1981, **30**, 817 (*rev*)
U.K. Pat., 2 133 002; *CA*, **101**, 231027 (*synth, isomer*)
Chen, T.M. *et al*, *J. Chromatogr.*, 1984, **314**, 495 (*resoln*)
Hammond, E.J. *et al*, *Gen. Pharmacol.*, 1985, **16**, 441 (*rev*)
Smithers, J.A. *et al*, *J. Chromatogr.*, 1985, **341**, 232 (*hplc*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 17030.

3-Amino-4-hydroxybutanoic acid **A-80081**



(*S*)-*form*

$C_4H_9NO_3$ M 119.120

(S)-form

*Lactone: 4-Aminodihydro-2(3*H*)-furanone. β-Amino-γ-butyrolactone*
$C_4H_7NO_2$ M 101.105
Mp 198-201° (as hydrobromide). $[\alpha]_D^{20}$ −42.6° (c, 1.08 in H_2O).

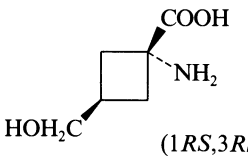
Lactone, N-*benzoyl:*
$C_{11}H_{11}NO_3$ M 205.213
Mp 123.5-126°. $[\alpha]_D^{20}$ −97.0° (c, 1.41 in $CHCl_3$).

(±)-form

Lactone: Mp 185-186° (as hydrochloride).

Chibnall, A.C. *et al*, *Biochem. J.*, 1958, **68**, 122 (*synth*)
McGarvey, G. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 4943 (*synth, pmr*)
Hvidt, T. *et al*, *Can. J. Chem.*, 1988, **66**, 779 (*synth, pmr, cmr*)

1-Amino-3-(hydroxymethyl)cyclobutanecarboxylic acid, 9CI **A-80082**



(1*RS*,3*RS*)-*form*

$C_6H_{11}NO_3$ M 145.158

(1RS,3RS)-form [116823-32-6]

trans-*form*

Synthetic. Cryst. Mp 255° dec.

(1RS,3SR)-form

cis-*form*

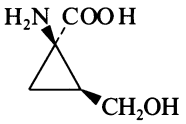
Minor component of the Costa Rican legume *Atelia herbert smithii* and of other *A.* and *Cyanthiostegia* spp. Cryst. (EtOH aq.). Mp 250-260° dec. (synthetic)(210°).

B,HCl: [109826-20-2].

Cryst.

Austin, G.N. *et al*, *Tetrahedron*, 1987, **43**, 1857 (*isol, ms, ir, pmr, cryst struct*)
Hughes, P. *et al*, *J. Org. Chem.*, 1988, **53**, 4793 (*synth, ir, pmr, cmr, ms*)
Fleet, G.W.J. *et al*, *Tetrahedron*, 1988, **44**, 2077 (*synth, ir, pmr, cmr, ms*)

1-Amino-2-(hydroxymethyl)cyclopropanecarboxylic acid A-80083



(1*R*,2*S*)-*form*

$C_5H_9NO_3$ M 131.131

Model for ethylene biogeneration in plants.

(1R,2S)-form

$[\alpha]_D^{25}$ +73.8° (c, 0.48 in H_2O).

(1S,2R)-form

Cryst. Mp 240° dec. $[\alpha]_D^{25}$ −74.5° (c, 0.184 in H_2O).

(1RS,2SR)-form

Cryst. (EtOH aq.). Mp 202° dec.

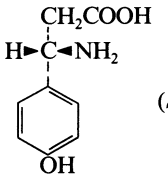
N-tert-*Butyloxycarbonyl:* Rhombs. Mp 151°.

Pirrung, M.C. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1301 (*synth, ir, pmr, cmr*)

3-Amino-3-(4-hydroxyphenyl)propanoic acid A-80084

*β-Amino-4-hydroxybemenepropanoic acid, 9CI. β-Amino-*p*-hydroxyhydrocinnamic acid, 8CI. β-Tyrosine. Isotyrosine*

[6049-54-3]



(*S*)-*form*

$C_9H_{11}NO_3$ M 181.191

(S)-form

D-*form*

B,HCl: [54732-46-6].

Needles (EtOH/EtOAc). $[\alpha]_D^{25}$ +7.8° (c, 1.67 in H_2O).

(±)-form

Cryst. (EtOH aq.). Mp 198°.

[52997-29-2, 54732-46-6, 73025-68-0, 73025-69-1]

Posner, T., *Justus Liebigs Ann. Chem.*, 1912, **389**, 1 (*synth*)
Profft, E. *et al*, *J. Prakt. Chem.*, 1965, **30**, 18 (*synth*)
Roncar, G. *et al*, *Biochemistry*, 1966, **5**, 2153.
Kurylo-Borowska, Z. *et al*, *Biochim. Biophys. Acta*, 1972, **264**, 1 (*biosynth*)
Chekhlov, A.N. *et al*, *Kristallografiya*, 1974, **19**, 981; (*Engl. Transl.*), 608 (*cryst struct*)
Parry, R.J. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 836 (*biosynth,abs config*)

4-Amino-4-(3-hydroxypropyl)-1,7-heptanediol A-80085

Bis-homotris

[116747-79-6]

$H_2NC(CH_2CH_2CH_2OH)_3$

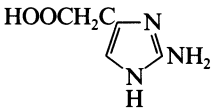
$C_{10}H_{23}NO_3$ M 205.297

Solid. Mp 108.5-109.8°. $Bp_{0.5}$ 220-235°.

Newkome, G.R. *et al*, *J. Org. Chem.*, 1988, **53**, 5552 (*synth, pmr, ir, cmr*)

2-Amino-4(5)-imidazoleacetic acid A-80086

[73086-08-5]



$C_5H_7N_3O_2$ M 141.129

Me ester: [110295-91-5].

$C_6H_9N_3O_2$ M 155.156

Oil (as trifluorocetate).

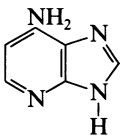
[110295-92-6]

Bouchet, M.-J. *et al*, *J. Med. Chem.*, 1987, **30**, 2222 (*synth, pmr, ms*)

7-Amino-3*H*-imidazo[4,5-*b*]pyridine A-80087

*1*H*-Imidazo[4,5-*b*]pyridin-7-amine, 9CI. 1-Deazaadenine*

[6703-44-2]



$C_6H_6N_4$ M 134.140

Cryst. (H_2O). Mp 258-260°.

B,HCl: [4261-04-5].

Needles (H_2O). Mp 327-329°.

B,2HCl: Cryst. Mp 325-328°.

Picrate: Mp >260°.

3-β-D-Ribofuranosyl: [14432-09-8]. *1-Deazaadenosine*

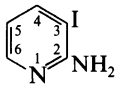
$C_{11}H_{14}N_4O_4$ M 266.256

Anti-leukaemic, shows other biological props. Cryst. (H_2O). Mp 262-263° dec. $[\alpha]_D^{25}$ −96.3° (c, 0.85 in DMF).

[57232-66-3]

Kögl, F. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1948, **67**, 29 (*synth*)
Jain, P.C. *et al*, *Indian J. Chem.*, 1966, **4**, 403 (*synth, deriv, uv, ir*)
De Roos, K.B. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1969, **88**, 1263; 1971, **90**, 654 (*deriv, synth, pmr, ir, uv*)
Itoh, T. *et al*, *J. Heterocycl. Chem.*, 1972, **9**, 465 (*deriv, synth, uv*)
Cristalli, G. *et al*, *J. Med. Chem.*, 1987, **30**, 1686 (*deriv, synth*)

2-Amino-3-iodopyridine, 8CI **A-80088**
3-Iodo-2-pyridinamine, 9CI
[104830-06-0]



$C_5H_5IN_2$ M 220.012
Needles (hexane). Mp 90-91.5°.
N-Me: [113975-23-8].
$C_6H_7IN_2$ M 234.039
Mp 50°. Bp_{14} 129°.

Sakamoto, T. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 4764 (*synth, pmr*)
Estel, L. *et al*, *J. Org. Chem.*, 1988, **53**, 2740 (*synth, pmr, ir, deriv*)

2-Amino-4-iodopyridine, 8CI **A-80089**
4-Iodo-2-pyridinamine, 9CI
$C_5H_5IN_2$ M 220.012
Cryst. (H_2O). Mp 163-164°.
Picrate: Cryst. (H_2O). Mp 253-254°.

Graf, R., *Chem. Ber.*, 1931, **64**, 21, 25.

2-Amino-5-iodopyridine, 8CI **A-80090**
5-Iodo-2-pyridinamine, 9CI
[20511-12-0]
$C_5H_5IN_2$ M 220.012
Needles (C_6H_6). Mp 130°.
Picrate: Yellow needles (EtOH or Me_2CO). Mp 240°.

Magidson, O.Yu. *et al*, *Ber.*, 1928, **58**, 114 (*synth*)
Caldwell, W.T. *et al*, *J. Am. Chem. Soc.*, 1944, **66**, 1479, 1481 (*synth*)
Shepherd, R.G. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 159 (*synth*)
Cumper, C.W.N., *J. Chem. Soc. B*, 1968, 649 (*uv*)
Jovanovic, M.V., *Heterocycles*, 1984, **22**, 1195 (*synth, pmr*)

2-Amino-6-iodopyridine, 8CI **A-80091**
6-Iodo-2-pyridinamine, 9CI
$C_5H_5IN_2$ M 220.012
Cryst. (Et_2O/pet.ether). Mp 106-106.5°.

Johnson, F., *J. Org. Chem.*, 1962, **27**, 2473 (*synth*)

3-Amino-5-iodopyridine, 8CI **A-80092**
5-Iodo-3-pyridinamine, 9CI
[25391-66-6]
$C_5H_5IN_2$ M 220.012
Cryst. (C_6H_6/pet.ether). Mp 71°.
Picrate: [25391-67-7].
Cryst. Mp 252° (225°).
N-Ac:
$C_7H_7IN_2O$ M 262.050
Cryst. Mp 202°.
N-Benzoyl:
$C_{12}H_9IN_2O$ M 324.120
Cryst. Mp 158°.

Plazek, E. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1938, **18**, 210, 215 (*synth*)
Batkowski, T., *Pol. J. Chem.* (*Rocz. Chem.*), 1969, **43**, 1623 (*synth, derivs*)

4-Amino-2-iodopyridine, 8CI **A-80093**
2-Iodo-4-pyridinamine, 9CI
$C_5H_5IN_2$ M 220.012
Cryst. (EtOH). Mp 98-99°.
N-oxide:
$C_5H_5IN_2O$ M 236.012
Cryst. (H_2O). Mp 110°.

Talik, T., *Pol. J. Chem.* (*Rocz. Chem.*), 1957, **31**, 569, 575 (*synth*)
Talik, Z., *Pol. J. Chem.* (*Rocz. Chem.*), 1961, **35**, 475 (*oxide*)

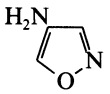
4-Amino-3-iodopyridine, 8CI **A-80094**
3-Iodo-4-pyridinamine, 9CI
$C_5H_5IN_2$ M 220.012
Needles (C_6H_6). Mp 76-77°.
Picrate: Mp 253° dec.
B,MeI: Cryst. (DMF or Et_2O). Mp 254.5-255°.

Profft, E. *et al*, *J. Prakt. Chem.*, 1959, **8**, 156, 163.
Talik, T., *Pol. J. Chem.* (*Rocz. Chem.*), 1962, **36**, 1049; 1963, **37**, 69.

5-Amino-2-iodopyridine, 8CI **A-80095**
6-Iodo-3-pyridinamine, 9CI
[29958-12-1]
$C_5H_5IN_2$ M 220.012
Needles (EtOH). Mp 132°.

Caldwell, W.T. *et al*, *J. Am. Chem. Soc.*, 1944, **66**, 1479, 1482 (*synth*)
Tomasik, P., *Pol. J. Chem.* (*Rocz. Chem.*), 1970, **44**, 509 (*synth*)

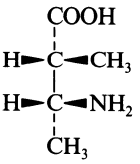
4-Aminoisoxazole **A-80096**
4-Isoxazolamine, 9CI
[108511-97-3]



$C_3H_4N_2O$ M 84.077
Dark-brown liq. V. sol. H_2O. Not obt. pure, clearly v. air-sensitive.
B,HCl: [108511-98-4].
Mp 160-163°.

Reiter, L.A., *J. Org. Chem.*, 1987, **52**, 2715 (*synth*)
Pascual, A., *Helv. Chim. Acta*, 1989, **72**, 556 (*synth, ir, pmr*)

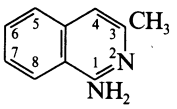
3-Amino-2-methylbutanoic acid **A-80097**
[32723-74-3]



$C_5H_{11}NO_2$ M 117.147
(2RS,3RS)-form
Needles ($MeOH/Et_2O$). Mp 221-222° dec.
[121054-31-7]

Estermann, H. *et al*, *Helv. Chim. Acta*, 1988, **71**, 1824 (*synth, ir, pmr, cmr*)

1-Amino-3-methylisoquinoline **A-80098**
3-Methyl-1-isoquinolinamine, 9CI



$C_{10}H_{10}N_2$ M 158.202

Cryst. (C_6H_6). Mp 130.5-131°.
B,HCl: Cryst. Mp 272-278°.
Bergstrom, F.W. *et al*, *J. Org. Chem.*, 1945, **10**, 479 (*synth*)

3-Amino-1-methylisoquinoline **A-80099**
1-Methyl-3-isoquinolinamine, 9CI
[15787-16-3]
$C_{10}H_{10}N_2$ M 158.202
Cryst. (EtOH). Mp 122-124°.
Picrate: [15896-92-1].
Cryst. Mp 232-233°.
Kametani, T. *et al*, *Chem. Pharm. Bull.*, 1967, **15**, 7 (*synth*)

3-Amino-4-methylisoquinoline **A-80100**
4-Methyl-3-isoquinolinamine, 9CI
[7697-66-7]
$C_{10}H_{10}N_2$ M 158.202
Pale yellow cryst. Mp 118-119°.
Win, H. *et al*, *J. Org. Chem.*, 1967, **32**, 59 (*synth, pmr, uv*)
Neumeyer, J.L., *J. Med. Chem.*, 1970, **13**, 613 (*synth*)

4-Amino-1-methylisoquinoline **A-80101**
1-Methyl-4-isoquinolinamine, 9CI
[104704-41-8]
$C_{10}H_{10}N_2$ M 158.202
Yellow prisms (Me_2CO/hexane).
Sawanishi, H. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 4564 (*synth, pmr*)

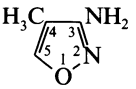
5-Amino-1-methylisoquinoline **A-80102**
1-Methyl-5-isoquinolinamine, 9CI
[20335-61-9]
$C_{10}H_{10}N_2$ M 158.202
Cryst. (C_6H_6). Mp 213-214°.
N-*Ac:*
$C_{12}H_{12}N_2O$ M 200.240
Cryst. (dioxan). Mp 226-227°.
N-*Me:* [53760-81-9].
$C_{11}H_{12}N_2$ M 172.229
Pale yellow prisms. (EtOAc/hexane). Mp 161.5-162.5°.
N,N-*Di-Me:* [84689-38-3].
$C_{12}H_{14}N_2$ M 186.256
Liq. $Bp_{0.05}$ 95-98°.
Agrawal, K.C. *et al*, *J. Med. Chem.*, 1968, **11**, 700.
Mooney, P.D. *et al*, *J. Med. Chem.*, 1974, **17**, 1145.
Tsuchiya, T. *et al*, *Chem. Pharm. Bull.*, 1982, **30**, 3757.

5-Amino-3-methylisoquinoline **A-80103**
3-Methyl-5-isoquinolinamine, 9CI
[54410-17-2]
Plates (EtOH aq.). Mp 219.5-221°.
Bergstrom, F.W. *et al*, *J. Org. Chem.*, 1945, **10**, 479 (*synth*)
Elderfield, R.C. *et al*, *J. Org. Chem.*, 1958, **23**, 435 (*synth*)
Buu-Hoi, N.P. *et al*, *J. Chem. Soc.*, 1964, 3924 (*synth*)

7-Amino-1-methylisoquinoline **A-80104**
1-Methyl-7-isoquinolinamine, 9CI
[31181-24-5]
$C_{10}H_{10}N_2$ M 158.202
Cryst. (C_6H_6). Mp 200-201°.
French, F.A. *et al*, *J. Med. Chem.*, 1970, **13**, 1117 (*synth*)

8-Amino-1-methylisoquinoline **A-80105**
1-Methyl-8-isoquinolinamine, 9CI
[31181-26-7]
$C_{10}H_{10}N_2$ M 158.202
Cryst. (C_6H_6). Mp 141-142°.
French, F.A. *et al*, *J. Med. Chem.*, 1970, **13**, 1117 (*synth*)

3-Amino-4-methylisoxazole **A-80106**
4-Methyl-3-isoxazolamine, 9CI
[1750-43-2]



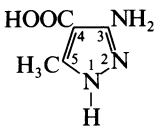
$C_4H_6N_2O$ M 98.104
Cryst. (C_6H_6/Et_2O). Mp 45-50°.
Klotzer, W. *et al*, *Monatsh. Chem.*, 1970, **101**, 1109 (*synth*)

4-Amino-3-methylisoxazole **A-80107**
3-Methyl-4-isoxazolamine, 9CI
$C_4H_6N_2O$ M 98.104
Yellow oil. d_4^{14} 1.172. Bp_{25} 130°. n_D^{14} 1.5069.
B,HCl: [108512-04-5].
Pink cryst. Mp 188-189°.
Quilico, A. *et al*, *Gazz. Chim. Ital.*, 1941, **71**, 327; 1942, **72**, 399 (*synth*)
Reiter, L.A., *J. Org. Chem.*, 1987, **52**, 2714 (*synth, ms, pmr*)

4-Amino-5-methylisoxazole **A-80108**
5-Methyl-4-isoxazolamine
[87988-94-1]
$C_4H_6N_2O$ M 98.104
Mp 25-31°.
B,HCl: [100499-66-9].
Cryst. Mp 184-195°.
Reiter, L.A., *J. Org. Chem.*, 1987, **52**, 2714 (*synth, ms, pmr*)
Pascual, A., *Helv. Chim. Acta*, 1989, **72**, 556 (*synth, ir, pmr*)

5-Amino-4-methylisoxazole **A-80109**
4-Methyl-5-isoxazolamine, 9CI
[35143-75-0]
$C_4H_6N_2O$ M 98.104
Matsumura, K. *et al*, *CA*, 1971, **76**, 85737n (*synth*)
Albrecht, H.A. *et al*, *J. Org. Chem.*, 1979, **44**, 4191 (*synth*)

3-Amino-5-methyl-1*H*-pyrazole-4-carboxylic acid, 9CI **A-80110**
5-Amino-3-methyl-4-pyrazolecarboxylic acid
[23286-64-8]



$C_5H_7N_3O_2$ M 141.129
Needles. Mp 124-125°.
Me ester: [23286-71-7].
$C_6H_9N_3O_2$ M 155.156
Microcryst. Mp 145-146.5°.
Et ester: [23286-70-6].
$C_7H_{11}N_3O_2$ M 169.183
Prisms. Mp 113°.

Et ester, monohydrate: Needles (H_2O). Mp 69°.

Et ester; B,HCl: [113270-87-4].
Cryst. Mp 188-189°.

Nitrile: [5453-07-6]. *2-Amino-3-cyano-4-methylpyrazole*
$C_5H_6N_4$ M 122.129
Mp 163°.

Beyer, H. *et al*, *Chem. Ber.*, 1956, **89**, 1652 (*synth, ester*)
Badger, G.M. *et al*, *Aust. J. Chem.*, 1965, **18**, 1267 (*synth, nitrile*)
Baba, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1969, **42**, 1653 (*synth*)

4-Amino-5-methyl-1*H*-pyrazole-3-carboxylic acid, 9CI — A-80111

[94993-81-4]

$C_5H_7N_3O_2$ M 141.129
Cryst. (H_2O). Mp 185-190° dec., Mp 208° dec.

B,HCl: Cryst. (H_2O). Mp 213-214°.

Hydrazide: [28668-09-9].
$C_5H_9N_5O$ M 155.159
Cryst. (2-Propanol). Mp 187.5-190°.

Et ester: [70015-75-7].
$C_7H_{11}N_3O_2$ M 169.183
Cryst. (C_6H_6). Mp 96-96.5°.

N-*Ac, Et ester:* [70015-77-9].
$C_9H_{13}N_3O_3$ M 211.220
Cryst. (EtOAc). Mp 176-177°.

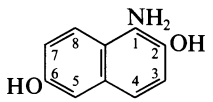
Amide:
$C_5H_8N_4O$ M 140.144
Cryst. (H_2O). Mp 209-211°.

Nitrile: [28745-14-4]. *4-Amino-3-cyano-5-methylpyrazole*
$C_5H_6N_4$ M 122.129
Cryst. (toluene). Mp 158-160°.

Musante, C. *et al*, *Gazz. Chim. Ital.*, 1947, **77**, 182 (*synth*)
Robins, R.K. *et al*, *J. Org. Chem.*, 1956, **21**, 833 (*synth*)
Long, R.A. *et al*, *J. Heterocycl. Chem.*, 1970, **7**, 863 (*nitrile, hydrazide*)
Takei, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 208 (*synth, esters*)

1-Amino-2,6-naphthalenediol, 8CI, 9CI — A-80112

2,6-Dihydroxy-1-naphthylamine. 1-Amino-2,6-dihydroxynaphthalene



$C_{10}H_9NO_2$ M 175.187

Di-Me ether: 2,6-Dimethoxy-1-naphthylamine. 1-Amino-2,6-dimethoxynaphthalene
$C_{12}H_{13}NO_2$ M 203.240
Orange needles (C_6H_6). Mp 189°.

Chakravarty, S. .N. *et al*, *J. Chem. Soc.*, 1937, 1859 (*synth*)

1-Amino-2,7-naphthalenediol, 8CI, 9CI — A-80113

Updated Entry replacing D-04799
2,7-Dihydroxy-1-naphthylamine

$C_{10}H_9NO_2$ M 175.187

O,O,N-Tri Ac:
$C_{16}H_{15}NO_5$ M 301.298
Cryst. Mp 183°.

Di-Me ether: [83011-60-3]. *2,7-Dimethoxy-1-naphthylamine*
$C_{12}H_{13}NO_2$ M 203.240
Cryst. (C_6H_6/ligroin); Needles (EtOH aq.). Mp 82-83°.

Di-Me ether, N-*Ac:*
$C_{14}H_{15}NO_3$ M 245.277
Cryst. (EtOH). Mp 179-180°.

Clausius, A., *Ber.*, 1890, **23**, 517.
Nietski, R. *et al*, *Ber.*, 1897, **30**, 1119.
Chakravarti, S.N. *et al*, *J. Chem. Soc.*, 1937, 1859 (*synth, deriv*)
Soffer, M.D. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3704 (*synth*)

2-Amino-1,4-naphthalenediol, 9CI, 8CI — A-80114

Updated Entry replacing D-04794
1,4-Dihydroxy-2-naphthylamine

[75539-34-3]

$C_{10}H_9NO_2$ M 175.187

O,O,N-*Tri-Ac:*
$C_{16}H_{15}NO_5$ M 301.298
Needles (AcOH). Mp 259-260°.

Di-Me ether: [50885-06-8]. *1,4-Dimethoxy-2-naphthylamine, 8CI*
$C_{12}H_{13}NO_2$ M 203.240
Plates (hexane or MeOH). Mp 100-101°.

Kehrmann, F., *Ber.*, 1894, **27**, 3337 (*synth*)
McCaustland, D.J. *et al*, *J. Med. Chem.*, 1973, **16**, 1311 (*synth*)
Ishii, H. *et al*, *Chem. Pharm. Bull.*, 1983, **31**, 4391 (*synth, ir*)
Malesani, G. *et al*, *J. Heterocycl. Chem.*, 1985, **22**, 1141 (*synth, pmr*)

2-Amino-1,6-naphthalenediol, 8CI, 9CI — A-80115

Updated Entry replacing D-04796
1,6-Dihydroxy-2-naphthylamine

[4826-64-6]

$C_{10}H_9NO_2$ M 175.187
Free base is very unstable.

O,O,N-*Tri-Ac:*
$C_{16}H_{15}NO_5$ M 301.298
Cryst. (ligroin or EtOH aq.). Mp 150°.

Fischer, E. *et al*, *J. Prakt. Chem.*, 1916, **94**, 5.

3-Amino-1,2-naphthalenediol, 8CI, 9CI — A-80116

Updated Entry replacing D-04801
3,4-Dihydroxy-2-naphthylamine

[58245-82-2]

$C_{10}H_9NO_2$ M 175.187
Cryst. (Et_2O or C_6H_6/EtOH). Mp 164°.

N-*Ac:*
$C_{12}H_{11}NO_3$ M 217.224
Mp 170° dec.

O,O-*Di-Ac:*
$C_{14}H_{13}NO_4$ M 259.261
Cryst. (AcOH). Mp >200° dec.

Di-Me ether: 3,4-Dimethoxy-2-naphthylamine
$C_{12}H_{13}NO_2$ M 203.240
Prisms (pet. ether). Mp 76°.

Ueno, A. *et al*, *Chem. Pharm. Bull.*, 1966, **14**, 129 (*synth, deriv*)
Greenland, H. *et al*, *Aust. J. Chem.*, 1975, **28**, 2655 (*synth, uv, ir, pmr*)

4-Amino-1,2-naphthalenediol, 8CI, 9CI — A-80117

Updated Entry replacing D-04800
3,4-Dihydroxy-1-naphthylamine

$C_{10}H_9NO_2$ M 175.187

N-*Ac:*
$C_{12}H_{11}NO_3$ M 217.224
Cryst. (H_2O). Mp 187° dec.

O,O,N-*Tri-Ac:*
$C_{16}H_{15}NO_5$ M 301.298
Cryst. (EtOH). Mp 206.5-207.5°.

Di-Me ether: [73168-34-0]. *3,4-Dimethoxy-1-naphthylamine*

$C_{12}H_{13}NO_2$ M 203.240
Cryst. (C_6H_6/hexane). Mp 140-142°.

Di-Me ether, N-Ac:
$C_{14}H_{15}NO_3$ M 245.277
Cryst. (C_6H_6). Mp 133-135°.

Kehrmann, F., *Ber.*, 1894, **27**, 3337.
Bogdanov, S.V. *et al*, *CA*, 1961, **55**, 11372b.
Archer, S. *et al*, *J. Med. Chem.*, 1980, **23**, 516.

4-Amino-1,3-naphthalenediol, 8CI, 9CI A-80118

Updated Entry replacing D-04798

2,4-Dihydroxy-1-naphthylamine. 2,4-Dihydroxy-1-naphthalenamine, 9CI

[31209-82-2]

$C_{10}H_9NO_2$ M 175.187
Mp 162°.

B,HCl: [30832-70-3].
Needles (dil. HCl).

O,O,N-Tri-Ac:
$C_{16}H_{15}NO_5$ M 301.298
Plates (C_6H_6). Mp 170-171° (155-156°).

Kehrmann, F. *et al*, *Chem. Ber.*, 1895, **28**, 345; 1896, **29**, 1415.
Lantz, R., *Bull. Soc. Chim. Fr.*, 1971, 249, 253.

4-Amino-1,5-naphthalenediol, 8CI, 9CI A-80119

4,8-Dihydroxy-1-naphthylamine. 4-Amino-1,5-dihydroxynaphthalene

$C_{10}H_9NO_2$ M 175.187

Di-Me ether: 4,8-Dimethoxy-1-naphthylamine. 4-Amino-1,5-dimethoxynaphthalene
$C_{12}H_{13}NO_2$ M 203.240
Leaflets (EtOH). Mp 160°.

Di-Me ether, N-Ac:
$C_{14}H_{15}NO_3$ M 245.277
Needles (EtOH). Mp 186°.

Thomson, R.H. *et al*, *J. Chem. Soc.*, 1947, 350 (*synth, deriv*)

4-Amino-1,7-naphthalenediol, 8CI, 9CI A-80120

4,6-Dihydroxy-1-naphthylamine. 1-Amino-4,6-dihydroxynaphthalene

[38410-19-4]

$C_{10}H_9NO_2$ M 175.187
Mp 178° dec.

O,O,N-Tribenzoyl:
$C_{31}H_{21}NO_5$ M 487.511
Mp 208°.

Jubault, M. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 1551 (*synth, deriv, ir*)

5-Amino-1,2-naphthalenediol, 8CI, 9CI A-80121

5,6-Dihydroxy-1-naphthylamine. 5-Amino-1,2-dihydroxynaphthalene

$C_{10}H_9NO_2$ M 175.187

Di-Me ether: 5,6-Dimethoxy-1-naphthylamine. 5-Amino-1,2-dimethoxynaphthalene
$C_{12}H_{13}NO_2$ M 203.240
Cryst. (EtOH). Mp 97-98°.

Sprenger, W.K. *et al*, *J. Org. Chem.*, 1966, **31**, 2402.

5-Amino-2,3-naphthalenediol A-80122

1-Amino-6,7-dihydroxynaphthalene

$C_{10}H_9NO_2$ M 175.187

Di-Me ether: [52401-42-0]. *6,7-Dimethoxy-1-naphthylamine. 1-Amino-6,7-dimethoxynaphthalene*
$C_{12}H_{13}NO_2$ M 203.240
Cryst. (EtOH). Mp 130°.

Di-Me ether, N-Ac:
$C_{14}H_{15}NO_3$ M 245.277
Cryst. (C_6H_6). Mp 185°.

Govindachari, T.R. *et al*, *J. Chem. Soc.*, 1955, 2534.
Kessar, S.V. *et al*, *Indian J. Chem.*, 1973, **11**, 1105 (*synth*)
Stermitz, F.R. *et al*, *J. Med. Chem.*, 1975, **18**, 708 (*synth*)

6-Amino-2,3-naphthalenediol, 8CI, 9CI A-80123

6,7-Dihydroxy-2-naphthylamine. 6-Amino-2,3-dihydroxynaphthalene

$C_{10}H_9NO_2$ M 175.187

Di-Me ether: [56517-29-4]. *6,7-Dimethoxy-2-naphthylamine. 6-Amino-2,3-dimethoxynaphthalene*
$C_{12}H_{13}NO_2$ M 203.240
Cryst. Mp 202-203°.

Stermitz, F.R. *et al*, *J. Med. Chem.*, 1975, **18**, 708 (*synth, deriv*)

6-Amino-1,2-napthalenediol, 8CI, 9CI A-80124

5,6-Dihydroxy-2-naphthylamine. 6-Amino-1,2-dihydroxynaphthalene

[21489-73-6]

$C_{10}H_9NO_2$ M 175.187

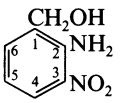
B,HCl: [21538-03-4].
Cryst. (MeOH/Et_2O). Mp 275-277° dec.

Di-Me ether: [23922-96-5]. *5,6-Dimethoxy-2-naphthylamine. 6-Amino-1,2-dimethoxynaphthalene*
$C_{12}H_{13}NO_2$ M 203.240
Prisms (EtOH). Mp 148.5-149.5°.

Sprenger, W.K. *et al*, *J. Med. Chem.*, 1969, **12**, 487 (*synth*)

2-Amino-3-nitrobenzyl alcohol A-80125

2-Amino-3-nitrobenzenemethanol, 9CI. 2-Hydroxymethyl-6-nitroaniline



$C_7H_8N_2O_3$ M 168.152

N-*Et:* [37637-56-2].
$C_9H_{12}N_2O_3$ M 196.205
Liq. $Bp_{0.1}$ 137-138°.

N-*Et, Et ether:* [37637-57-3].
$C_{11}H_{16}N_2O_3$ M 224.259
Orange liq. $Bp_{0.2}$ 135-140°.

Gawron, O. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5396 (*synth, uv, ms, ir*)

2-Amino-6-nitrobenzyl alcohol A-80126

2-Amino-6-nitrobenzenemethanol, 9CI. 2-Hydroxymethyl-3-nitroaniline

[98451-51-5]

$C_7H_8N_2O_3$ M 168.152
Yellow needles (CH_2Cl_2/pet. ether). Mp 96.5-97.5°.

Hewgill, F.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1305 (*synth, pmr*)

3-Amino-2-nitrobenzyl alcohol A-80127

3-Amino-2-nitrobenzenemethanol, 9CI. 3-Hydroxymethyl-2-nitroaniline

$C_7H_8N_2O_3$ M 168.152

N-*Et:* [37637-53-9].

$C_9H_{12}N_2O_3$ M 196.205
Cryst. (H_2O). Mp 105-105.5°.

Gawron, O. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5396 (*synth, uv, ms, ir*)

3-Amino-4-nitrobenzyl alcohol A-80128

3-Amino-4-nitrobenzenemethanol, 9CI. 5-Hydroxymethyl-2-nitroaniline

[37637-55-1]

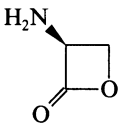
$C_7H_8N_2O_3$ M 168.152
Yellow needles (C_6H_6). Mp 139-140.5°.

N-*Et:* [37637-54-0].
$C_9H_{12}N_2O_3$ M 196.205
Orange needles (H_2O). Mp 95-96°.

Gawron, O. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5396 (*synth, ir, uv, ms*)

3-Amino-2-oxetanone A-80129

α-Amino-β-propiolactone. Serine β-lactone



(*S*)-*form*

$C_3H_5NO_2$ M 87.078

(*S*)-*form*

L-form
Salts descr. react with nucleophiles to give optically pure amino acids.

Trifluoroacetate salt: [112839-94-8].
Unstable, used immediately.

4-Methylbenzenesulfonate: [112839-95-9].
Cryst. (DMF/Et_2O). $[\alpha]_D^{25}$ −15.9° (c, 2.2 in DMF). Darkens from 135°, dec. >173°.

N-tert-*Butyloxycarbonyl:* [98541-64-1].
$C_8H_{13}NO_4$ M 187.195
Cryst. Mp 119.5-120.5° dec. $[\alpha]_D^{22}$ −26.7° (c, 1 in MeCN).

Arnold, L.D. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 7105; 1987, **109**, 4649; 1988, **110**, 2237 (*synth, ir, pmr, cmr, ms, use*)

8-Amino-7-oxononanoic acid, 9CI A-80130

[4707-58-8]

$H_3CCH(NH_2)CO(CH_2)_5COOH$

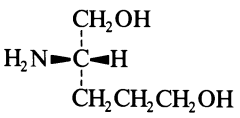
$C_9H_{17}NO_3$ M 187.238
Isol. from *Penicillium chrysogeum* as a biotin intermediate.
Cryst. (EtOH/Et_2O). Mp 133-134°.

Suyama, T. *et al*, *CA*, 1964, **60**, 4013 (*synth*)
Iwahara, S. *et al*, *Agric. Biol. Chem.*, 1966, **30**, 304.
Eisenburg, M.A. *et al*, *Biochemistry*, 1970, **9**, 108.

2-Amino-1,5-pentanediol, 9CI A-80131

Updated Entry replacing A-02457
Glutaminediol

[21926-01-2]



(*S*)-*form*

$C_5H_{13}NO_2$ M 119.163

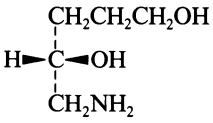
(*S*)-*form* [21946-71-4]

$Bp_{1.5}$ 150-159°.

Oxalate: Mp 111-113°. $[\alpha]_D^{20}$ +10.0° (c, 2.0 in H_2O).

Jutisz, M. *et al*, *Bull. Soc. Chim. Biol.*, 1954, **36**, 117; *CA*, **48**, 10494 (*synth*)
Herbrandson, H.F. *et al*, *J. Med. Chem.*, 1969, **12**, 620 (*synth*)
Prasad, B. *et al*, *Indian J. Chem.*, 1974, **12**, 290 (*synth*)
Danklmaier, J. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 851 (*synth, cmr*)

5-Amino-1,4-pentanediol A-80132



$C_{15}H_{13}NO_2$ M 239.273

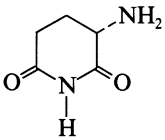
(*S*)-*form*

$Bp_{0.02}$ 90-100° (bath) . $[\alpha]_D^{20}$ +2.2° (c, 1.5 in AcOH).

Danklmeier, J. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 1149 (*synth, cmr*)

3-Amino-2,6-piperidinedione, 9CI A-80133

2-Aminoglutarimide. Glutamic acid imide



(*S*)-*form*

$C_5H_8N_2O_2$ M 128.130

(*S*)-*form*

B,HBr: [118061-00-0].
Mp 279° dec.

Poloński, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 639 (*synth, cd, uv, pmr*)

3-Amino-2-formyl-2-propenoic acid A-80134

$H_2NCH{=}C(CHO)COOH$

$C_4H_5NO_3$ M 115.088
Derivs are useful synthetic intermeds.

Me ester: [64944-80-5]. *Methyl 3-amino-2-formyl-2-propenoate*
$C_5H_7NO_3$ M 129.115
Cryst. (MeCN). Mp 115°.

N-*Me, Me ester:* [107195-10-8]. *Methyl 2-formyl-3-methylamino-2 propenoate*
$C_6H_9NO_3$ M 143.142
Cryst. Mp 69°.

N-tert-*Butyl, Me ester:* [82100-23-0]. *Methyl 3-*tert-*butylamino-2-formyl-2-propenoate*
$C_9H_{15}NO_3$ M 185.222
Cryst. Mp 55°.

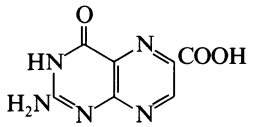
N-Ph, Me ester: Methyl 2-formyl-3-phenylamino-2-propenoate
$C_{11}H_{11}NO_3$ M 205.213
Cryst. Mp 73°.

Tietze, L.F. *et al*, *Chem. Ber.*, 1989, **122**, 83.

2-Amino-4(3*H*)-pteridinone-6-carboxylic acid A-80135

2-Amino-1,4-dihydro-4-oxo-6-pteridinecarboxylic acid, 9CI. Pterin-6-carboxylic acid

[948-60-7]



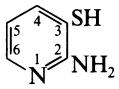
$C_7H_5N_5O_3$ M 207.148
Cream cryst. Mp >300°.

Sato, N. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1737.

2-Amino-3-pyridinethiol, 9CI A-80136

2-Amino-3-mercaptopyridine

[110402-20-5]



$C_5H_6N_2S$ M 126.182
Has antibacterial props. Intermed. for pharmaceuticals.

Ger. Pat., 3 545 124; 3 545 097; *CA*, **107**, 134219q; **107**, 154346g (*synth, use*)

4-Amino-3-pyridinethiol A-80137

4-Amino-3-mercaptopyridine

[52334-54-0]

$C_5H_6N_2S$ M 126.182
Semisolid.

Picrate: Yellow needles (EtOH). Mp 228° dec.

Takahashi, T. *et al*, *Chem. Pharm. Bull.*, 1956, **4**, 216 (*synth*)
Smith, K. *et al*, *Chem. Ind.* (*London*), 1988, 302 (*synth*)

6-Amino-3-pyridinethiol A-80138

2-Amino-5-mercaptopyridine

[68559-17-1]

$C_5H_6N_2S$ M 126.182

$SnCl_2$/HCl salt: Cryst. (conc. HCl). Mp 265-267°.

S-*Et:* [71167-00-5]. *5-Ethylthio-2-pyridinamine, 9CI. 2-Amino-5-ethylthiopyridine*
$C_7H_{10}N_2S$ M 154.235
Mp 20°. Bp_{15} 166-169°.

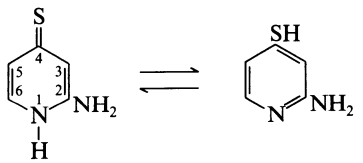
S-*Et, picrate:* [71167-01-6].
Cryst. (EtOH). Mp 238-240°.

Ger. Pat., 2 812 914, (1978); *CA*, **90**, 6397q (*synth, props*)
Gold'farb, Ya.L. *et al*, *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1979, **15**, 514 (*synth, deriv*)
U.S. Pat., 4 221 796, (1980); *CA*, **94**, 192328y (*synth, use, deriv*)

2-Amino-4(1*H*)-pyridinethione, 9CI A-80139

2-Amino-4-pyridinethiol. 2-Amino-4-mercaptopyridine

[38240-25-4]



$C_5H_6N_2S$ M 126.182

Intermed. for cephalosporins. Cryst. (Me_2CO). Mp 223° dec.

Picrate: Yellow cryst. (H_2O). Mp >185° dec.

S-*Me:* [38240-26-5]. *4-Methylthio-2-pyridinamine, 9CI. 2-Amino-4-methylthiopyridine*
$C_6H_8N_2S$ M 140.209
Cryst. (cyclohexane). Mp 122-123°.

[59243-52-6, 59243-57-1, 59243-61-7, 65872-14-2]

Barlin, G.B., *J. Chem. Soc., Perkin Trans.* 2, 1972, 1459 (*synth, uv*)

3-Amino-4(1*H*)-pyridinethione, 9CI A-80140

3-Amino-4-pyridinethiol. 3-Amino-4-mercaptopyridine

[89002-13-1]

$C_5H_6N_2S$ M 126.182
Intermed. for cephalosporins. Pale yellow granules (H_2O). Sol. aq. alkalies. Mp 213° dec.

S-*Me:* [38240-24-3]. *4-Methylthio-3-pyridinamine. 3-Amino-4-methylthiopyridine*
$C_6H_8N_2S$ M 140.209
Yellow needles (MeOH)(as picrate). Mp 173-174° (165-166°) (picrate).

S-*Et: 4-Ethylthio-3-pyridinamine. 3-Amino-4-ethylthiopyridine*
$C_7H_{10}N_2S$ M 154.235
Needles (EtOH)(as hydrochloride). Mp 213° dec. (hydrochloride).

N-*Ac*,S-*Me:*
$C_8H_{10}N_2OS$ M 182.246
Granules $+\frac{1}{2}H_2O$ (Me_2CO). Mp 109° approx.

[38240-23-2, 59243-59-3, 59243-62-8]

Takahashi, T. *et al*, *Chem. Pharm. Bull.*, 1954, **2**, 196; 1955, **3**, 356 (*synth, derivs*)
Barlin, G.B., *J. Chem. Soc., Perkin Trans.* 2, 1972, 1459 (*synth, uv, props*)

5-Amino-2(1*H*)-pyridinethione, 8CI A-80141

5-Amino-2-pyridinethiol. 5-Amino-2-mercaptopyridine

[27885-56-9]

$C_5H_6N_2S$ M 126.182
Intermed. for diazo dyes. Golden needles (H_2O). Sol. hot H_2O. Mp 172-175°. Readily oxidises in air to disulfide.

N-*Ac:* [27885-57-0].
$C_7H_8N_2OS$ M 168.219
Bright yellow cryst. (H_2O). Mp 244-246°.

S-*Me:* [29958-08-5]. *6-Methylthio-3-pyridinamine, 9CI. 5-Amino-2-methylthiopyridine, 8CI*
$C_6H_8N_2S$ M 140.209
Brown-yellow or light brown needles (C_6H_6/pet. ether or cyclohexane). Mp 71-72°.

S-*Me, picrate:* Cryst. (EtOH). Mp 127-129°.

S-*Et:* [52025-15-7]. *6-Ethylthio-3-pyridinamine. 5-Amino-2-ethylthiopyridine*
$C_7H_{10}N_2S$ M 154.235
Viscous yellow oil. Bp 126°.

S-*Et; B,2HCl:* [96592-07-3].
Small blunt needles (EtOH). Mp 175-176°.

N-*Ac*, S-*Me:* [29958-16-5].
$C_8H_{10}N_2OS$ M 182.246
Cryst. (H_2O). Mp 155-155.5°.

[59243-51-5, 59315-59-2, 96592-06-2]

Rath, C., *Justus Liebigs Ann. Chem.*, 1931, **487**, 105 (*synth*)
Caldwell, W.T. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 1695 (*synth, props, deriv*)
Takahashi, T. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1942, **62**, 140; 1945, **65**, 14 (*synth, derivs*)

Forrest, H.S. *et al*, *J. Chem. Soc.*, 1948, 1939 (*synth, deriv*)
Tomasik, P., *Pol. J. Chem.* (*Rocz. Chem.*), 1970, **44**, 509 (*synth, props, deriv*)
Seydel, J.K., *J. Med. Chem.*, 1971, **14**, 724 (*pmr, deriv*)
Barlin, G.B., *J. Chem. Soc., Perkin Trans.* 2, 1972, 1459 (*synth, uv, derivs*)
Akers, H.A. *et al*, *Can. J. Chem.*, 1987, **65**, 1364 (*synth, ir*)

6-Amino-2(1*H*)-pyridinethione, 9CI — A-80142

6-Amino-2-pyridinethiol, 9CI. 2-Amino-6-mercaptopyridine

[38240-17-4]

$C_5H_6N_2S$ M 126.182

Cryst. (Me_2CO). Mp 198°. Prob. yellow, though no colour mentioned.

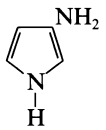
S-*Me:* [38240-18-5]. *6-Methylthio-2-pyridinamine, 9CI. 2-Amino-6-methylthiopyridine*
$C_6H_8N_2S$ M 140.209
Cryst. (cyclohexane). Mp 67-68°.

[59315-52-5, 59315-60-5]

Barlin, G.B., *J. Chem. Soc., Perkin Trans.* 2, 1972, 1459 (*synth, uv, deriv*)
Kwiatkowski, J.S. *et al*, *Acta Phys. Pol. A*, 1976, **49**, 393; *CA*, **84**, 179475t (*uv*)

3-Aminopyrrole — A-80143

1H-Pyrrole-3-amine



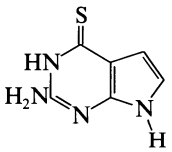
$C_4H_6N_2$ M 82.105

*1,N³-Di-*tert*-butyl:* [117203-10-8]. *1-*tert*-Butyl-3-(*tert*-butylamino)-1H-pyrrole*
$C_{12}H_{22}N_2$ M 194.319
$Bp_{0.01}$ 50°.

tom Dieck, H. *et al*, *Chem. Ber.*, 1989, **122**, 129 (*synth, ir, pmr, cmr*)

2-Aminopyrrolo[2,3-*d*]pyrimidine-4-thione — A-80144

7-Deaza-6-thioguanine



$C_6H_6N_4S$ M 166.206

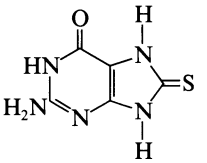
7-(2-Deoxy-β-D-ribofuranosyl): [104291-18-1]. *2'-Deoxy-7-deaza-6-thioguanosine*
$C_{11}H_{14}N_4O_3S$ M 282.323
Pale yellow needles (H_2O). Mp 196-210° dec. (>200°).

Seela, F. *et al*, *Justus Liebigs Ann. Chem.*, 1987, 15.
Ramasany, K. *et al*, *Tetrahedron Lett.*, 1987, **28**, 5107.

2-Amino-1,7,8,9-tetrahydro-2-thioxo-6*H*-purin-6-one, 9CI — A-80145

8-Mercaptoguanine, 8CI. 2-Amino-6-hydroxy-8-mercaptopurine

[6324-72-7]



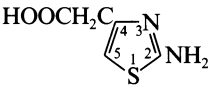
$C_5H_5N_5OS$ M 183.193

[28128-40-7]

Elion, G.B. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 1898 (*synth*)
Holmes, R.E. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1242 (*synth*)

2-Amino-4-thiazoleacetic acid — A-80146

[29676-71-9]



$C_5H_6N_2O_2S$ M 158.181

Mod. active plant growth regulator. Mp 121-122° dec. (130°).

HBF_4 salt: [110295-78-8].
Cryst. Mp 180-185°.

Et ester:
$C_7H_{10}N_2O_2S$ M 186.234
Mp 92-94°.

Steude, M., *Justus Liebigs Ann. Chem.*, 1891, **261**, 22 (*synth*)
Garraway, J.L., *Pestic. Sci.*, 1970, **1**, 240 (*props*)
Bouchet, M.-J. *et al*, *J. Med. Chem.*, 1987, **30**, 2222 (*synth, pmr*)

2-Amino-5-thiazoleacetic acid — A-80147

$C_5H_6N_2O_2S$ M 158.181

HBF_4 salt: [110295-79-9].
Mp 215° dec.

Et ester:
$C_7H_{10}N_2O_2S$ M 186.234
Plates (C_6H_6/pet. ether or $CHCl_3$/pet. ether). Mp 100-101°.

Et ester, picrate: Yellow needles (EtOH). Mp 204-205° dec.

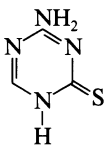
Amide:
$C_5H_7N_3OS$ M 157.196
Cryst. Mp 174-175° dec.

Mory, R. *et al*, *Helv. Chim. Acta*, 1950, **33**, 405 (*deriv, synth*)
Bouchet, M.-J. *et al*, *J. Med. Chem.*, 1987, **30**, 2222 (*synth, pmr*)

4-Amino-1,3,5-triazine-2(1*H*)-thione, 9CI — A-80148

4-Amino-1,2-dihydro-1,3,5-triazine-2-thione

[36469-86-0]



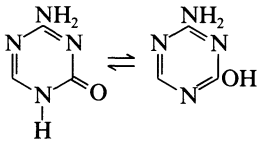
$C_3H_4N_4S$ M 128.157

Cryst. Mp >330°.

Niedballa, V. *et al*, *J. Org. Chem.*, 1974, **39**, 3672 (*synth, uv, pmr*)

4-Amino-1,3,5-triazin-2(1*H*)-one, 9CI A-80149

*4-Amino-*s*-triazin-2-ol. 2-Amino-4-hydroxy-*s*-triazine. 5-Azacytosine*



$C_3H_4N_4O$ M 112.091
Microcryst. powder. Insol. org. solvs. Mp >350° dec.

B,HCl: [16352-14-0].
Solid. Mp >350° (cryst. change at 250°).

1-(2,3-Dideoxy-β-D-ribofuranosyl): [107036-52-2]. *2′,3′-Dideoxy-5-azacytidine*
$C_8H_{12}N_4O_3$ M 212.208
Solid. Mp 247° dec.

*4-*N*-Me:* [16352-16-2].
$C_4H_6N_4O$ M 126.118
Cryst. (H_2O). Mp 310-311°.

*1,4-*N*-Di-Me:* [16352-08-2].
$C_5H_8N_4O$ M 140.144
Cryst. Mp 270-271°.

*4,4-*N*-Di-Me:* [16352-15-1].
$C_5H_8N_4O$ M 140.144
Cryst. (MeOH). Mp 268-269°.

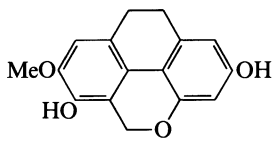
*1,4,4-*N*-Tri-Me:* [3391-73-9].
$C_6H_{10}N_4O$ M 154.171
Cryst. (MeOH). Mp 201-202°.

2-Me ether: [1122-73-2]. *2-Amino-4-methoxy-1,3,5-triazine*
$C_4H_6N_4O$ M 126.118
Cryst. (C_6H_6). Mp 188-189°.

[4040-10-2]

Grundmann, C. *et al*, *Chem. Ber.*, 1954, **87**, 19 (*synth*)
Piškala, A., *Collect. Czech. Chem. Commun.*, 1967, **32**, 3966, 4271 (*synth, derivs*)
Hartenstein, R. *et al*, *J. Org. Chem.*, 1967, **32**, 1653 (*synth*)
Niedballa, V. *et al*, *J. Org. Chem.*, 1974, **39**, 3672 (*synth*)
Kim, C.-H. *et al*, *J. Med. Chem.*, 1987, **30**, 862 (*deriv, synth, pmr, ms*)

Amoenumin A-80150



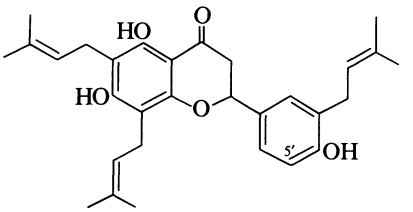
$C_{16}H_{14}O_4$ M 270.284
Constit. of *Dendrobium amoenum*. Cryst. (MeOH). Mp 120°.

Veerraju, P. *et al*, *Phytochemistry*, 1989, **28**, 950.

Amorilin A-80151

Updated Entry replacing A-20156

4′,5,7-Trihydroxy-3′,6,8-triprenylflavanone. Euchrenone a_3
[83474-69-5]



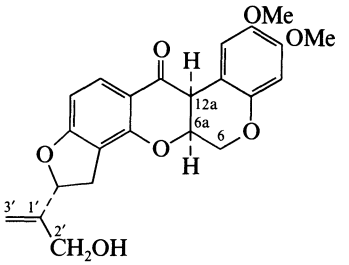
$C_{30}H_{36}O_5$ M 476.611
Constit. of *Amorpha fruticosa* and *Euchresta japonica*. Oil or pale-yellow powder (hexane). Mp 70-72°.

Rózsa, Z. *et al*, *Heterocycles*, 1982, **19**, 1793.
Mizuno, M. *et al*, *Phytochemistry*, 1988, **27**, 1831 (*isol*)

Amorphigenin A-80152

Updated Entry replacing A-02757

8′-Hydroxyrotenone
[4208-09-7]



$C_{23}H_{22}O_7$ M 410.423
Various numbering schemes have been used for the side-chain (here numbered 1′, 2′, 3′). Constit. of *Amorpha fruticosa* and of *Dalbergia monetaria*. Cryst. ($C_6H_6/CHCl_3$, $EtOH/CHCl_3$ or Me_2CO aq.). Mp 196-197°. $[\alpha]_D^{20}$ −125.6° (c, 2.04 in $CHCl_3$).

▷ VL1575000.

O-*β-D-Glucopyranoside:*
$C_{29}H_{32}O_{12}$ M 572.565
Isol. from seeds of *A.* spp. and *D. monetaria*. Mp 164°. $[\alpha]_D^{20}$ −122° (c, 0.1 in EtOH).

2′-(6-O-α-L-Arabinopyranosyl-β-D-glucopyranoside): [4207-90-3]. ***Amorphin***
$C_{34}H_{40}O_{16}$ M 704.680
Glycoside from *A. fruticosa*. Needles. Mp 154-155°. $[\alpha]_D^{18.5}$ −123.6° (c, 1.1 in MeOH), $[\alpha]_D^{24.5}$ −87.9° (c, 2.55 in Py).

1′,3′-Dihydro: [30462-22-7]. ***Dihydroamorphigenin.*** *22,23-Dihydro-24-hydroxyrotenone*
$C_{23}H_{24}O_7$ M 412.438
Isol. from seeds of *A. fruticosa*. Mp 189-190°.

1′,3′-Dihydro, 1′-hydroxy: [29360-12-1]. ***Amorphigenol***
$C_{23}H_{24}O_8$ M 428.438
Constit. of *A.* spp. Needles. Mp 195-196°. $[\alpha]_D^{20}$ −124° (c, 0.47 in EtOH).

1′,3′-Dihydro, 1′-hydroxy, 1′-O-β-D-glucopyranoside: [29360-13-2]. *Amorphigenol glucoside*
$C_{29}H_{34}O_{13}$ M 590.580
Isol. from seeds of *A. fruticosa*. Faintly yellow cryst. Mp 189-192° dec. $[\alpha]_D^{20}$ −94.7° (c, 1.3 in MeOH).

1′,3′-Dihydro, 2′-O-[α-L-arabinopyranosyl(1→6)-β-D-glucopyranoside]: [53947-91-4]. ***Amorphol***

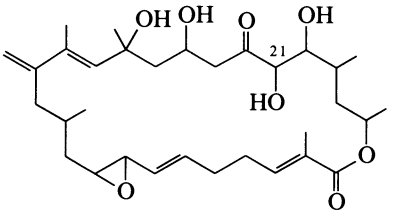
$C_{34}H_{42}O_{16}$ M 706.696
Constit. of the roots of *A. fruticosa*. Yellowish powder. Mp 159-162° dec. $[\alpha]_D^{22}$ −96.6° (c, 2.07 in MeOH). Incorr. descr. as a dioxin deriv. in CA owing to a drawing error in the paper.

6a,12a-Didehydro: [29444-01-7]. ***Dehydroamorphigenin***
$C_{23}H_{20}O_7$ M 408.407
Isol. from *A.* spp. seeds. Pale-yellow needles. Mp 228-5-229.5° dec. $[\alpha]_D^{19}$ −50.8° (c, 0.83 in $CHCl_3$).

Claisse, J. *et al*, *J. Chem. Soc.*, 1964, 6023 (*isol, struct, bibl*)
Kasymov, A.U. *et al*, *Khim. Prir. Soedin.*, 1968, **4**, 326; 1970, **6**, 197; 1972, **8**, 115; 1974, **10**, 464; *Chem. Natl. Compd.*, 277, 192, 109, 470 (*Amorphigenol glucoside, Dihydroamorphigenin, Amorphol, Amorphigenol*)
Crombie, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 1285; 1975, 1497 (*biosynth, pmr*)
Crombie, L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 1143, 1144; 1986, 1063 (*biosynth*)

Amphidinolide B — A-80153

Updated Entry replacing A-70205
[110786-78-2]

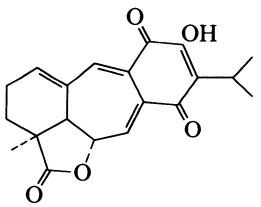


$C_{32}H_{50}O_8$ M 562.742
Macrolide antibiotic. Isol. from *Amphidinium* sp. Shows antitumour props. Amorph. $[\alpha]_D^{25}$ −45° (c, 1 in $CHCl_3$).

21-Epimer: ***Amphidinolide D***
$C_{32}H_{50}O_8$ M 562.742
Isol. from an *A.* sp. Shows antitumour props. Amorph. solid. $[\alpha]_D^{30}$ −30° (c, 0.5 in $CHCl_3$).

Ishibashi, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1127 (*isol, struct*)
Kobayashi, J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1036 (*isol, pmr, cmr*)

Anastomosine — A-80154

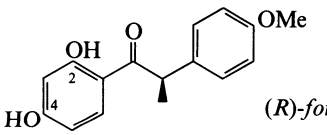


$C_{20}H_{20}O_5$ M 340.375
Constit. of *Salvia anastomosans*. Yellow cryst. Mp 207-215°. $[\alpha]_D^{20}$ +426.5° (c, 0.034 in Py).

Sánchez, C. *et al*, *Phytochemistry*, 1989, **28**, 1681.

Angolensin — A-80155

Updated Entry replacing A-02947
1-(2,4-Dihydroxyphenyl)-2-(4-methoxyphenyl)-1-propanone, 9CI



(*R*)-*form*

$C_{16}H_{16}O_4$ M 272.300

(***R***)-***form*** [4842-48-2]
Constit. of *Pericopsis elata, P. mooniana, Pterocarpus angolensis, P. erinaceus* and *P. indica*. Prisms (pet. ether). Mp 120-121°. $[\alpha]_D^{24}$ −114° (c, 1 in $CHCl_3$).

2-Me ether: [58822-06-3]. ***2-O-Methylangolensin***
$C_{17}H_{18}O_4$ M 286.327
Constit. of *Pericopsis elata*. Oil. $[\alpha]_D^{24}$ +5.3° ($CHCl_3$).

4-Me ether: Mp 62°. $[\alpha]_D^{24}$ −142° (c, 2 in $CHCl_3$).

2,4-Di-Me ether: Mp 49°. $[\alpha]_D^{24}$ +26° ($CHCl_3$).

(***S***)-***form***
4-Me ether: [75946-85-9]. ***4-O-Methylangolensin***
$C_{17}H_{18}O_4$ M 286.327
Isol. from heartwood of *P. angolensis*. Needles (MeOH). Mp 28-30°.

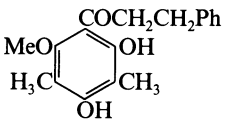
(±)-***form***
Constit. of *Pericopsis mooniana*. Mp 86-88°.

2,4-Di-Me ether: Mp 70°.

King, F.E. *et al*, *J. Chem. Soc.*, 1952, 1920 (*isol, struct*)
Foxall, C.D. *et al*, *J. Chem. Soc.*, 1963, 5573 (*isol, struct*)
Ollis, W.D. *et al*, *Aust. J. Chem.*, 1965, **18**, 1787 (*abs config*)
Clark-Lewis, J.W. *et al*, *Aust. J. Chem.*, 1965, **18**, 1791 (*abs config*)
Aggarwal, S.K. *et al*, *Indian J. Chem.*, 1970, **8**, 478 (*synth*)
Fitzgerald, M.A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 186 (2-*O*-Methylangolensin)
Bezuidenhondt, B.C.B. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 2179 (4-*O*-Methylangolensin)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

Angoletin — A-80156

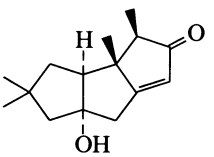
1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone, 9CI. 2′,4′-Dihydroxy-6′-methoxy-3′,5′-dimethyldihydrochalcone
[76444-55-8]



$C_{18}H_{20}O_4$ M 300.354
Isol. from *Uvaria angolensis*. Cryst. ($CHCl_3$/hexane). Mp 74-76°.

Hufford, C.D. *et al*, *Phytochemistry*, 1980, **19**, 2036 (*isol, uv, pmr, struct, cmr*)

Anhydroarthrosporone — A-80157



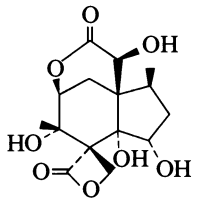
$C_{15}H_{22}O_2$ M 234.338
Metab. of an unidentified fungus (UAMH 4262). Cryst. (Et_2O/hexane). Mp 118-119°. $[\alpha]_D$ +62° (c, 2 in $CHCl_3$).

Amouzou, E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1042 (*isol, pmr*)

Anisatin A-80158

Updated Entry replacing A-03011

[5230-87-5]



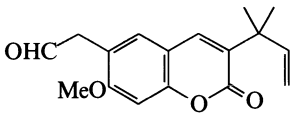
$C_{15}H_{20}O_8$ M 328.318

Isol. from seeds of *Illicium anisatum*. Cryst. (H_2O). Mp 227-228°. $[\alpha]_D^{25}$ −27° (c, 2 in dioxan).

▷ Convulsant poison.

Lane, J.F. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 3211 (*isol*)
Yamada, K. *et al*, *Tetrahedron Lett.*, 1965, 4797 (*struct*)
Wong, M.G. *et al*, *Aust. J. Chem.*, 1988, **41**, 1071 (*cryst struct, pmr*)

Anisocoumarin A A-80159

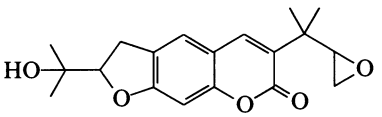


$C_{17}H_{18}O_4$ M 286.327

Constit. of *Clausena anisata*. Yellow oil.

Ngadjui, B.T. *et al*, *Phytochemistry*, 1989, **28**, 585.

Anisocoumarin C A-80160

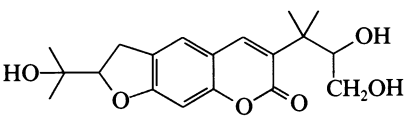


$C_{19}H_{22}O_5$ M 330.380

Constit. of *Clausena anisata*. Oil. $[\alpha]_D^{25}$ +15.5° (c, 1.1 in $CHCl_3$).

Ngadjui, B.T. *et al*, *Phytochemistry*, 1989, **28**, 585.

Anisocoumarin D A-80161



$C_{19}H_{24}O_6$ M 348.395

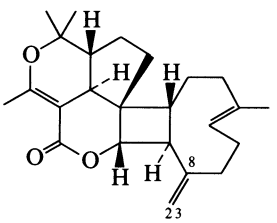
Constit. of *Clausena anisata*. Cryst. (MeOH). Mp 210-211°. $[\alpha]_D^{25}$ +20.5° (c, 1.2 in MeOH).

Ngadjui, B.T. *et al*, *Phytochemistry*, 1989, **28**, 585.

Antheliolide A A-80162

Updated Entry replacing A-70213

[114915-36-5]



$C_{24}H_{32}O_3$ M 368.515

Novel acetoacetylated diterpenoid skeleton. Constit. of soft coral *Anthelia glauca*. Mp 180°. Exists as mixt. of two conformers.

8ξ,23-Epoxide: [114933-19-6]. ***Antheliolide B***

$C_{24}H_{32}O_4$ M 384.514

Constit. of *A. glauca*. Oil.

Green, D. *et al*, *Tetrahedron Lett.*, 1988, **29**, 1605 (*isol*)
Smith, A.B. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3363 (*cryst struct*)

9-Anthracenesulfonic acid, 9Cl A-80163

Updated Entry replacing A-03081

[22582-76-9]

$C_{14}H_{10}O_3S$ M 258.297

V. sol. H_2O. Dec. in acid soln.

Na salt: [17213-01-3].

Gold plates.

Chloride: [53973-96-9].

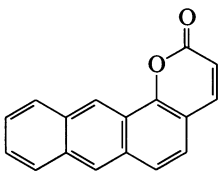
$C_{14}H_9ClO_2S$ M 276.743

Used as protecting group in peptide synth. Yellow solid. Mp 133°. Unstable.

Yura, S., *Kogyo Kagaku Zasshi*, 1941, **44**, 731; *CA*, **42**, 6793 (*synth*)
Zorn, H., *Monatsh. Chem.*, 1967, **98**, 2406 (*synth, ir*)
Arzeno, H.B. *et al*, *Synthesis*, 1988, 32 (*chloride*)

2*H*-Anthra[1,2-*b*]pyran-2-one A-80164

[6812-13-1]



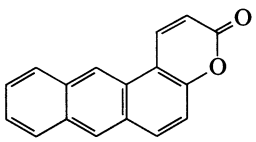
$C_{17}H_{10}O_2$ M 246.265

Cryst. Mp 223-225°.

Harvey, R.G. *et al*, *J. Org. Chem.*, 1988, **53**, 3936 (*synth, pmr*)

3*H*-Anthra[2,1-*b*]pyran-3-one A-80165

[6706-90-7]

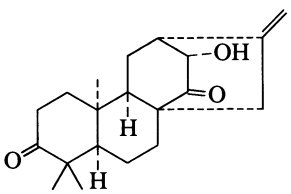


$C_{17}H_{10}O_2$ M 246.265

Cryst. Mp 198-199°.

Harvey, R.G. *et al*, *J. Org. Chem.*, 1988, **53**, 3936 (*synth, pmr*)

Antiquorin A-80166



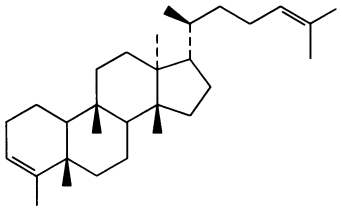
$C_{20}H_{28}O_3$ M 316.439

Constit. of *Euphorbia antiquorum*. Cryst. ($CHCl_3$/MeOH). Mp 163-164°. $[\alpha]_D^{15}$ +70° (c, 0.1 in MeOH).

Zhi-Da, M. *et al*, *Phytochemistry*, 1989, **28**, 553.

3,24-Aonenadiene A-80167

3,21-Aonenadiene

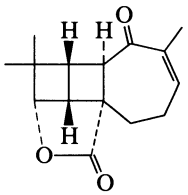


$C_{30}H_{50}$ M 410.725

3,24-Aonenadiene corresponds to the normal numbering system. Constit. of rhizomes of *Polypodioides niponica*. Cryst. Mp 89-91°. $[\alpha]_D^{23}$ +8.9° (c, 0.8 in $CHCl_3$).

Arai, Y. *et al*, *Tetrahedron Lett.*, 1989, **30**, 7209.

Aquatolide A-80168



$C_{15}H_{18}O_3$ M 246.305

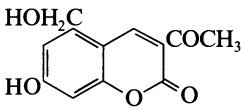
Constit. of *Asteriscus aquaticus*. Cryst. Mp 142-143°. $[\alpha]_D$ +66.3° (c, 0.45 in $CHCl_3$).

San Feliciano, A. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2851.

Armillarisin A A-80169

3-Acetyl-5-(hydroxymethyl)-7-hydroxy-2H-1-benzopyran-2-one, 9CI. 3-Acetyl-5-hydroxymethyl-7-hydroxycoumarin

[56696-47-5]



$C_{12}H_{10}O_5$ M 234.208

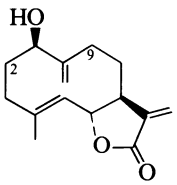
Isol. from *Armillariella tabescens*. Mp 245-246°.

Anon, *CA*, 1975, **82**, 1919m, 40463c.

Artemorin A-80170

Updated Entry replacing A-20211

[64845-92-7]



$C_{15}H_{20}O_3$ M 248.321

Constit. of *Artemisia verlotorum*. Cryst. (CH_2Cl_2/Et_2O). Mp 120-121°. $[\alpha]_D$ +89°.

2α-Hydroxy: ***2α-Hydroxyartemorin***

$C_{15}H_{20}O_4$ M 264.321

Constit. of *A. hispanica*. Needles (EtOH). Mp 220-221°.

9β-Hydroxy: ***9β-Hydroxyartemorin***

$C_{15}H_{20}O_4$ M 264.321

Constit. of *Inula heterolepis*. Gum.

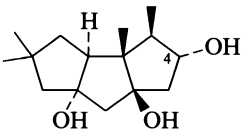
Geissman, T.A., *Phytochemistry*, 1970, **9**, 2377 (*isol*)

El-Feraly, F.S. *et al*, *Tetrahedron Lett.*, 1977, 1973 (*struct*)

Bohlmann, F. *et al*, *Phytochemistry*, 1982, **21**, 1166 (*isol*)

Sanz, J.F. *et al*, *Phytochemistry*, 1989, **28**, 2163 (*isol, pmr*)

Arthrosporol A-80171



$C_{15}H_{26}O_3$ M 254.369

Metab. of an unidentified fungus (UMAH 4262). Cryst. (Et_2O). Mp 163-164°. $[\alpha]_D$ −29° (c, 2 in $CHCl_3$).

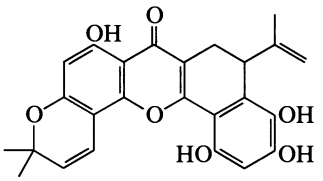
4-Ketone: ***Arthrosporone***

$C_{15}H_{24}O_3$ M 252.353

Metab. of fungus UAMH 4262. Cryst. (Et_2O/hexane). Mp 139-141°. $[\alpha]_D$ −140.8° (c, 0.9 in $CHCl_3$).

Amouzou, E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1042 (*isol, pmr*)

Artobiloxanthone A-80172

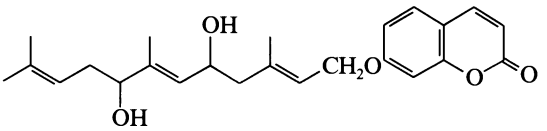


$C_{25}H_{22}O_7$ M 434.445

Constit. of *Artocarpus nobilis*. Yellow solid. Mp 162-164°.

Sultanbawa, M.U.S. *et al*, *Phytochemistry*, 1989, **28**, 599.

Asacoumarin A A-80173

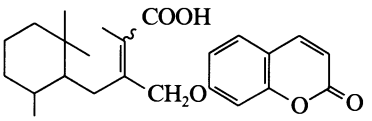


$C_{24}H_{30}O_5$ M 398.498

Constit. of *Ferula assa-foetida*. Oil. $[\alpha]_D$ +7° (c, 0.7 in $CHCl_3$).

Kazimoto, T. *et al*, *Phytochemistry*, 1989, **28**, 1761.

Asacoumarin B A-80174

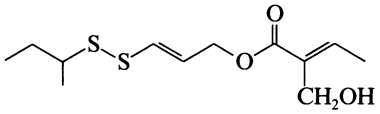


$C_{24}H_{30}O_5$ M 398.498

Constit. of *Ferula assa-foetida*. Amorph. powder. $[\alpha]_D$ −13.3° (c, 0.4 in $CHCl_3$).

Kajimoto, T. *et al*, *Phytochemistry*, 1989, **28**, 1761.

Asadisulphide A-80175

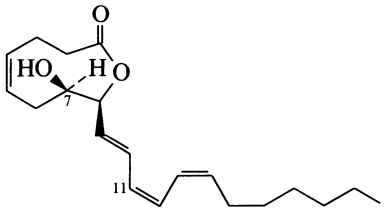


$C_{12}H_{20}O_3S_2$ M 276.420
Constit. of *Ferula assa-foetida*. Oil. $[\alpha]_D$ +24° (c, 0.4 in $CHCl_3$).

Kazimoto, T. *et al*, *Phytochemistry*, 1989, **28**, 1761.

Ascidiatrienolide A A-80176

[122752-22-1]



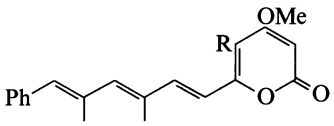
$C_{20}H_{30}O_3$ M 318.455
Constit. of *Didemnum candidum*. $[\alpha]_D$ −14.8° (c, 4.5 in $CHCl_3$).

7-Epimer: [122799-22-8]. ***Ascidiatrienolide B***
$C_{20}H_{30}O_3$ M 318.455
Constit. *D. candidum*. $[\alpha]_D$ −4.1° (c, 3.4 in $CHCl_3$).

11E-Isomer: [122799-23-9]. ***Ascidiatrienolide C***
$C_{20}H_{30}O_3$ M 318.455
Constit. of *D. candidum*. $[\alpha]_D$ −10.6° (c, 11.3 in $CHCl_3$).

Lindquist, N. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2735.

Asnipyrone A A-80177



R = CH_3

$C_{21}H_{22}O_3$ M 322.403
Metab. of *Aspergillus niger*. Yellow cryst. (EtOH). Mp 161-163°.

Guang-yi, L. *et al*, *Heterocycles*, 1989, **28**, 899.

Asnipyrone B A-80178

As Asnipyrone A, A-80177 with

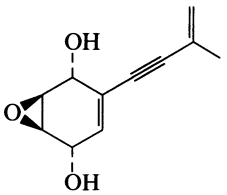
R = H

$C_{20}H_{20}O_3$ M 308.376
Metab. of *Aspergillus niger*. Yellow cryst. ($MeOH/CH_2Cl_2$). Mp 158-160°.

Guang-yi, L. *et al*, *Heterocycles*, 1989, **28**, 899.

Asperpentyne A-80179

[119483-44-2]

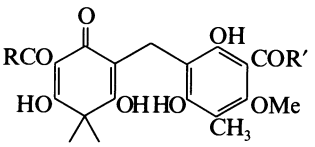


$C_{11}H_{12}O_3$ M 192.214
Metab. of *Aspergillus duricaulis*. Oil.

Mühlenfeld, A. *et al*, *Phytochemistry*, 1988, **27**, 3853.

Aspidins A-80180

Updated Entry replacing A-03572



Aspidin AA, R = R′ = CH_3
AB, R = CH_3, R′ = $CH_2CH_2CH_3$
PB, R = CH_2CH_3, R′ = $CH_2CH_2CH_3$
BB, R = R′ = $CH_2CH_2CH_3$

The suffix letters derive from the acyl side-chains (A = acetyl, P = propionyl, B = butyryl). Constits. of *Dryopteris* spp. ferns, also from *Aspidium* spp.

▷ GU5505000.

Aspidin AA [53526-70-8]
$C_{21}H_{24}O_8$ M 404.416
Constit. of *D. gymnospora*. Yellow needles (hexane). Mp 135-136°.

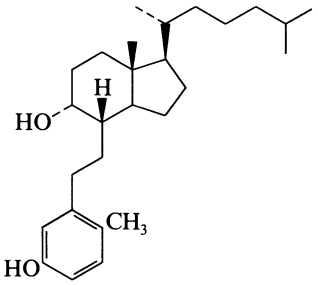
Aspidin AB [19489-46-4]
$C_{23}H_{28}O_8$ M 432.469
Mp 117-120°.

Aspidin BB [584-28-1]
Aspidin. Polystichin. Yellow polystichum acid
$C_{25}H_{32}O_8$ M 460.523
Pale-yellow cryst. (EtOH). Mp 125°.

Di-Ac: Needles and prisms (MeOH). Mp 108°.

Mitteldorf, R. *et al*, *Chem. Ber.*, 1956, **89**, 2595 (*synth*)
Aebi, A. *et al*, *Helv. Chim. Acta*, 1957, **40**, 569 (*struct*)
Huhtikangas, A. *et al*, *Acta Chem. Scand.*, 1972, **26**, 89 (*ms*)
Hisada, S. *et al*, *Phytochemistry*, 1974, **13**, 655 (*isol*, *struct*)
Widen, C.-J. *et al*, *Helv. Chim. Acta*, 1976, **59**, 1725 (*isol*, *pmr*)

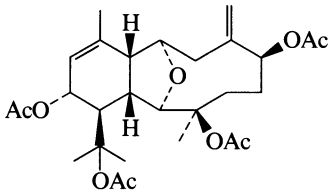
Astrogorgiadiol A-80181



$C_{27}H_{44}O_2$ M 400.643
Metab. of gorgonian *Astrogorgia* sp. Inhibits cell division in fertilised starfish eggs. Solid. $[\alpha]_D$ −16.4° (c, 0.058 in $CHCl_3$).

Fusetani, N. *et al*, *Tetrahedron Lett.*, 1989, **30**, 7079.

Astrogorgin A-80182

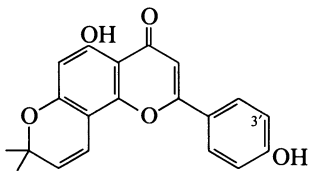


$C_{28}H_{40}O_9$ M 520.619
Metab. of gorgonian *Astrogorgia* sp. Inhibits cell division in fertilised starfish eggs. $[\alpha]_D$ −118° (c, 0.064 in $CHCl_3$).

Fusetani, N. *et al*, *Tetrahedron Lett.*, 1989, **30**, 7079.

Atalantoflavone A-80183

[119309-02-3]



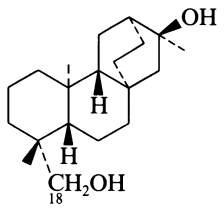
$C_{20}H_{16}O_5$ M 336.343
Constit. of *Atalantia racemosa*. Yellow needles (Me_2CO/hexane). Mp 289-290°.

3′-Methoxy: [106055-12-3]. ***Racemoflavone***
$C_{21}H_{18}O_6$ M 366.370
Constit. of *A. racemosa*. Yellow cryst. (Me_2CO/hexane). Mp 236-237°.

Banerji, A. *et al*, *Phytochemistry*, 1988, **27**, 3637 (*isol, struct, synth*)

ent-16α,18-Atisanediol A-80184

[118243-65-5]



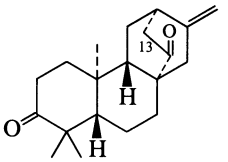
$C_{20}H_{34}O_2$ M 306.487
Constit. of *Xylopia aromatica*. Cryst. (hexane). Mp 160-162°. $[\alpha]_D^{25}$ −45° (c, 0.02 in $CHCl_3$).

18-Carboxylic acid: [118243-66-6]. **ent-*16α-Hydroxy-18-atisanoic acid***
$C_{20}H_{32}O_3$ M 320.471
Constit. of *X. aromatica*.

18-Carboxylic acid, Me ester: Cryst. (hexane). Mp 140-142°. $[\alpha]_D^{25}$ −24° (c, 0.01 in $CHCl_3$).

Moraes, M.P.L. *et al*, *Phytochemistry*, 1988, **27**, 3205.

ent-16-Atisene-3,14-dione A-80185



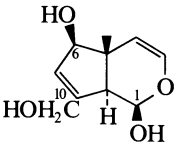
$C_{20}H_{28}O_2$ M 300.440
Constit. of *Euphorbia fidjiana*. Cryst. Mp 160-164°. $[\alpha]_D^{25}$ +5.5° (c, 0.02 in $CHCl_3$).

13R-Hydroxy: **ent-*13R-hydroxy-16-atisene-3,14-dione***
$C_{20}H_{28}O_3$ M 316.439
Constit. of *E. fidjiana*. Cryst. Mp 175-177°. $[\alpha]_D^{25}$ +44° (c, 0.03 in $CHCl_3$).

Lal, A.R. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3205 (*cryst struct*)

Aucubigenin A-80186

Updated Entry replacing A-10277
[64274-28-8]



$C_9H_{12}O_4$ M 184.191
Oil.

1-O-β-D-Glucopyranoside: [479-98-1]. *Aucubin. Aucuboside*
$C_{15}H_{22}O_9$ M 346.333
Constit. of *Plantago lanceolata* and *Aucuba japonica*. Cryst. + $1H_2O$ (EtOH aq.). Mp 181°. $[\alpha]_D^{21}$ −171.4° (H_2O).

1-O-β-Cellobioside:
$C_{21}H_{32}O_{14}$ M 508.475
Constit. of *Odontites verna*. Amorph. powder. $[\alpha]_D^{25}$ −92.0° (c, 0.7 in MeOH).

1-O-β-Gentiobioside:
$C_{21}H_{32}O_{14}$ M 508.475
Constit. of *O. verna*. Cryst. (EtOH). Mp 180-181°. $[\alpha]_D^{25}$ −45° (c, 1.5 in MeOH).

1-O-β-D-(2′-Benzoylglucopyranosyl): 2′-O-Benzoylaucubin
$C_{22}H_{26}O_{10}$ M 450.441
Constit. of *O. verna*. Amorph. powder. $[\alpha]_D^{25}$ −124.8° (c, 0.4 in MeOH).

6-Epimer, 1-O-β-D-glucopyranoside: 6-Epiaucubin
$C_{15}H_{22}O_9$ M 346.333
Constit. of *Tecoma chrysantha*. Amorph. powder. $[\alpha]_D^{25}$ −58.9° (c, 0.7 in MeOH).

1-O-β-D-Glucopyranoside,1′-O-(p-hydroxybenzoyl): ***Agnuside.*** *Agnoside*
$C_{22}H_{26}O_{11}$ M 466.441

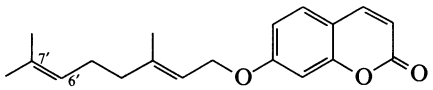
Isol. from *Vitex agnus-castus*, *V. regundo*, *V. trifolia*, *V. lucens* and other V. spp., also *Rhinanthus* spp. Cryst. (H_2O). Mp 146°. $[\alpha]_D^{20}$ −91.5° (EtOH).

Hänsel, R. *et al*, *Phytochemistry*, 1965, **4**, 19 (*Agnaside*)
Bianco, A. *et al*, *Tetrahedron*, 1977, **33**, 847; 1982, **38**, 362.
Bianco, A. *et al*, *Gazz. Chim. Ital.*, 1981, **111**, 91, 479; 1982, **112**, 227 (*isol*)
Damtoft, S., *Phytochemistry*, 1983, **22**, 1929 (*biosynth*)

Auraptene† A-80187

*7-(3,7-Dimethyl-2,6-octadienyl)oxy-2*H*-1-benzopyran-2-one, 9CI. O-Geranylumbelliferone. Feronialactone. 7-Geranyloxycoumarin*

[495-02-3]



$C_{19}H_{22}O_3$ M 298.381
Isol. from *Citrus aurantium*, *Feronia elephantum*, *Aegle marmelos*, *Libanotis intermedia* and others. Prisms (EtOH). Mp 68°.

*6′*R*,7-Epoxy:* [36414-00-3]. ***6′,7′-Epoxyaurapten.*** *7-[[5-(3,3-Dimethyloxiranyl)-3-methyl-2-pentenyl]oxy]-2*H*-1-benzopyran-2-one, 9CI*
$C_{19}H_{22}O_4$ M 314.380
Isol. from *Aster yunnanensis*. Oil or cryst. Mp 55-57.5°. $[\alpha]_D^{22}$ +21° ($CHCl_3$).

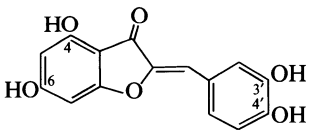
Kariyone, T. *et al*, *Chem. Pharm. Bull.*, 1959, **1**, 119 (*struct, synth, bibl*)
Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1968, **717**, 186 (*isol, uv, pmr, struct, deriv*)
Coates, R.M. *et al*, *Tetrahedron*, 1970, **26**, 5699 (*synth*)
Yamada, S. *et al*, *Tetrahedron Lett.*, 1976, **29**, 2557 (*synth, abs config, deriv*)

Aureusidin A-80188

Updated Entry replacing A-10282

*2-[(3,4-Dihydroxyphenyl)methylene]-4,6-dihydroxy-3(2*H*)-benzofuranone, 9CI. 3′,4,4′,6-Tetrahydroxyaurone. Cernuine*

[480-70-6]



$C_{15}H_{10}O_6$ M 286.240
Aglucone from *Antirrhinum majus*, also isol. from *Citrus medica*. Present in various members of the Gesneriaceae. Deep-yellow cryst. + $1H_2O$ (MeOH aq.). Mp 270°, Mp 295° dec. (double Mp).

Tetra-Ac: Yellow needles (pet. ether). Mp 188-189°.

4-O-β-D-Glucopyranoside: [480-69-3]. ***Cernuoside***
$C_{21}H_{20}O_{11}$ M 448.382
Pigment from *Oxalis cernua*, also present in *Chirita micromusa*, *Limonium bonduellii* and *Petrocosmea kerrii*. Yellow cryst. (EtOH aq.). Mp 250-258°. $[\alpha]_D^{30}$ −13° (Py).

6-O-β-D-Glucopyranoside: [633-15-8]. ***Aureusin***
$C_{21}H_{20}O_{11}$ M 448.382
Constit. of *A. majus*, also in *Antirrhinum nuttalianum* and *Linaria maroccana*. Needles (EtOAc) (as hepta-Ac). Mp 264.5-265.5° (as hepta-Ac).

6-Me ether: [54826-89-0]. ***Rengasin.*** *3′,4,4′-Trihydroxy-6-methoxyaurone*
$C_{16}H_{12}O_6$ M 300.267
Constit. of *Melanorrhea* spp. heartwood. Golden-yellow cryst. Mp 314-316° dec.

Tetra-Me ether: Greenish-yellow needles (MeOH aq.). Mp 173° (169-170°).

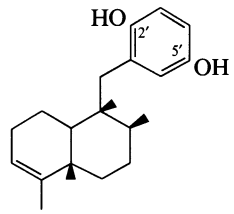
[38216-54-5]

Geissman, T.A. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 5725; 1955, **77**, 4622 (*isol, struct*)
Farkas, L. *et al*, *Chem. Ber.*, 1961, **94**, 2221; 1964, **97**, 1044; 1969, **49**, 2221 (*synth*)
Batterham, T.J. *et al*, *Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Harborne, J.B., *Phytochemistry*, 1966, **5**, 111, 589 (*occur*)
Hastings, J.S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 2128 (*pmr, struct*)
Deshmukh, S.W. *et al*, *Indian J. Chem.*, 1974, **12**, 893 (*synth*)

Avarol A-80189

Updated Entry replacing A-10285

[55303-98-5]



Absolute configuration

$C_{21}H_{30}O_2$ M 314.467
Constit. of *Dysidea avara*. Cryst. ($CHCl_3$). Mp 148-150°. $[\alpha]_D$ +6.1°.

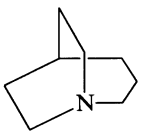
5′-Ac:
$C_{23}H_{32}O_3$ M 356.504
Constit. of *D. avara*. Cryst. (Et_2O/hexane). Mp 151-152°. $[\alpha]_D^{25}$ +11° (c, 3.1 in $CHCl_3$).

2′,5′-Quinone: [55303-99-6]. ***Avarone***
$C_{21}H_{28}O_2$ M 312.451
From *D. avara*. Oil.

Minale, L. *et al*, *Tetrahedron Lett.*, 1974, 3401 (*isol*)
de Rosa, S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 1408 (*struct*)
Sarma, A.S. *et al*, *J. Org. Chem.*, 1982, **47**, 1727 (*synth*)
Crispino, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 646 (*isol, pmr, cmr*)

1-Azabicyclo[3.2.2]nonane A-80190

[283-20-5]



$C_8H_{15}N$ M 125.213
Cryst. Mp 129°. Bp 170°.

Picrate: Yellow needles (EtOH). Mp 288-289°.

Prelog, V. *et al*, *Justus Liebigs Ann. Chem.*, 1937, **532**, 83 (*synth*)
Ruggles, C.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5692 (*synth, spectra*)

1-Azabicyclo[3.3.1]nonane, 9CI, 8CI A-80191

Updated Entry replacing A-10287

Isogranatanine

[280-77-3]

$C_8H_{15}N$ M 125.213

Needles. Mp 114°. Bp_{18} 100-105°. Hygroscopic.

B,HCl: Cryst. (EtOH/Et_2O). Mp >350°.

Picrate: Yellow cryst. (EtOH). Mp 282.5-283° dec.

Prelog, V. *et al*, *Chem. Ber.*, 1939, **72**, 1319 (*synth*)
Miyano, S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 313 (*synth, pmr, cmr*)

3-Azetidinone A-80192

C_3H_5NO M 71.079

Claimed syntheses prior to 1988 were prob. erroneous.

B,HCl: [17557-84-5].
Solid. Sol. H_2O. Mp 110-140°. Cont. ca 20% MeOH.

1-Benzoyl: [25566-02-3].
$C_{10}H_9NO_2$ M 175.187
Cryst.

Baumann, H. *et al*, *Helv. Chim. Acta*, 1988, **71**, 1035 (*synth, ir, pmr*)

3-Azido-1-butyne A-80193

[118723-97-0]

$$HC{\equiv}CCH(N_3)CH_3$$

$C_4H_5N_3$ M 95.104

Liq.

Banert, K., *Chem. Ber.*, 1989, **122**, 911 (*synth, ir, pmr, cmr*)

4-Azido-2-butyn-1-ol A-80194

[118723-98-1]

$$N_3CH_2C{\equiv}CCH_2OH$$

$C_4H_5N_3O$ M 111.103

Liq.

▷ Potentially explosive.

Banert, K., *Chem. Ber.*, 1989, **122**, 911 (*synth, ir, pmr, cmr*)

1-Azido-4-chloro-2-butyne A-80195

[119720-88-6]

$$N_3CH_2C{\equiv}CCH_2Cl$$

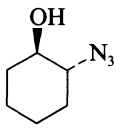
$C_4H_4ClN_3$ M 129.548

Liq.

Banert, K., *Chem. Ber.*, 1989, **122**, 1175.

2-Azidocyclohexanol A-80196

[71559-13-2]



$C_6H_{11}N_3O$ M 141.172

(1RS,2RS)-form [10027-78-8]

(±)-trans-*form*
Liq. $Bp_{1.5}$ 70-71°.

Ac: [10027-85-7].
$C_8H_{13}N_3O_2$ M 183.210
Oil.

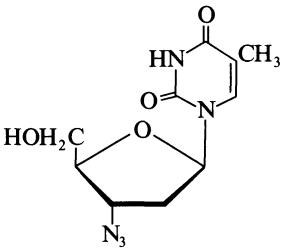
Van der Werf, C.A. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 1231 (*synth, ir*)
Cambie, R.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 840 (*synth, ir, pmr*)
Mereyala, H.B. *et al*, *Helv. Chim. Acta*, 1986, **69**, 415 (*synth*)

3′-Azido-3′-deoxythymidine, 9CI A-80197

Updated Entry replacing A-50371

3′-Azidothymidine. ***Zidovudine,*** **BAN, INN, USAN.** *BW A509U. Retrovir. AZT*

[30516-87-1]



$C_{10}H_{13}N_5O_4$ M 267.244

Antiviral agent active exclusively against retroviruses, esp. AIDS virus and leukaemias. Drug of choice (1986) for AIDS treatment. Needles (Et_2O). Mp 106-112°, Mp 119-121° (after drying).

Horowitz, J.P. *et al*, *J. Org. Chem.*, 1964, **29**, 2076 (*synth, uv*)
Lin, T.-S. *et al*, *J. Med. Chem.*, 1978, **21**, 109 (*synth*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 18797.
Mitsuya, H. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1985, **82**, 7096 (*pharmacol*)
Dyer, I. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 767 (*cryst struct*)
Van Roey, P. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2277 (*cryst struct*)
Fleet, G.W.J. *et al*, *Tetrahedron*, 1988, **44**, 625 (*synth*)

2-Azido-1,3-diiodopropane A-80198

$$(ICH_2)_2CHN_3$$

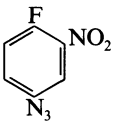
$C_3H_5I_2N_3$ M 336.902

Liq.

Sehgal, R.K. *et al*, *J. Med. Chem.*, 1987, **30**, 1626 (*synth, ir, pmr*)

4-Azido-1-fluoro-2-nitrobenzene, 9CI A-80199

[28166-06-5]



$C_6H_3FN_4O_2$ M 182.114

Used for affinity labelling of antibodies. Orange or straw needles (pet. ether). Mp 53-55° (52°).

▷ Explosive when dry.

Fleet, G.W.J. *et al*, *Nature (London)*, 1969, **224**, 511 (*synth, use*)
Fleet, G.W.J. *et al*, *Biochem. J.*, 1972, **128**, 499 (*synth, uv, haz*)
Gabizon, R. *et al*, *J. Biol. Chem.*, 1982, **257**, 15145 (*ms*)

2-Azido-3-iodo-1-propanol A-80200

[109122-91-0]

$ICH_2CH(N_3)CH_2OH$

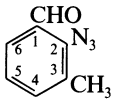
$C_3H_6IN_3O$ M 227.004

(±)-*form*
Yellowish liq.

Sehgal, R.K. *et al*, *J. Med. Chem.*, 1987, **30**, 1626 (*synth, pmr, ir*)

2-Azido-3-methylbenzaldehyde A-80201

[113302-67-3]



$C_8H_7N_3O$ M 161.163
Pale yellow oil.

Cuevas, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 2055 (*synth, ir, pmr, ms*)

2-Azido-5-methylbenzaldehyde A-80202

[113302-66-2]

$C_8H_7N_3O$ M 161.163
Yellow solid. Mp 55.5-56.5°.

Cuevas, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 2055 (*synth, ir, pmr, ms*)

3-Azido-3-methyl-1-butyne A-80203

[118723-88-9]

$N_3C(CH_3)_2C{\equiv}CH$

$C_5H_7N_3$ M 109.130
Liq.

▷ Potentially explosive.

Banert, K., *Chem. Ber.*, 1989, **122**, 911 (*synth, ir, pmr, cmr, ms*)

1-Azido-1-propanol A-80204

$H_3CCH_2CH(OH)N_3$

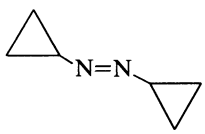
$C_3H_7N_3O$ M 101.108

Me ether: [111238-42-7]. *1-Azido-1-methoxypropane*
$C_4H_9N_3O$ M 115.135
Liq. Bp_{625} 100-105°.

Hassner, A. *et al*, *J. Org. Chem.*, 1988, **53**, 22 (*synth, ir, pmr, ms*)

Azocyclopropane A-80205

Updated Entry replacing A-20255
Dicyclopropyldiazene
[78331-66-5]



(*E*)-*form*

$C_6H_{10}N_2$ M 110.158

N-*Oxide:* [33425-51-3]. *Azoxycyclopropane*
$C_6H_{10}N_2O$ M 126.158
Bp_{40} 104-107°, Bp_{10} 80-83°. Geom. isom. not determined.

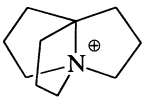
(*E*)-*form* [80201-75-8]
Bp 139°.

(*Z*)-*form* [80201-76-9]
Mp 38-39.5°.

Iversen, P.E., *Chem. Ber.*, 1971, **104**, 2195 (*oxide, synth, ir*)
Engel, P.S. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 7689 (*synth, spectra*)
Engel, P.S. *et al*, *J. Org. Chem.*, 1988, **53**, 4748 (*synth, pmr, cmr, uv, ms, props*)

1-Azoniatricyclo[3.3.3.0]undecane A-80206

*Tetrahydro-1*H,*5*H-*4,7*a-*propanopyrrolizinium, 9CI. 1-Azonia[3.3.3]propellane*



$C_{10}H_{18}N^{\oplus}$ M 152.259

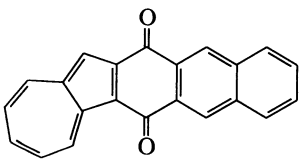
Chloride: [116747-82-1].
$C_{10}H_{18}ClN$ M 187.712
Solid. Mp >350°.

Bromide:
$C_{10}H_{18}BrN$ M 232.163
Prisms. Mp >350°.

Šorm, F. *et al*, *Collect. Czech. Chem. Commun.*, 1954, **19**, 298 (*synth, ir*)
Newkome, G.R. *et al*, *J. Org. Chem.*, 1988, **53**, 5552 (*synth, pmr, ir, pmr*)

Azuleno[1,2-*b*]anthracene-6,13-dione, 9CI A-80207

*Anthra[2,3-*a]*azulene-6,13-dione*
[87121-88-8]



$C_{22}H_{12}O_2$ M 308.336
Green cryst. Mp >310°.

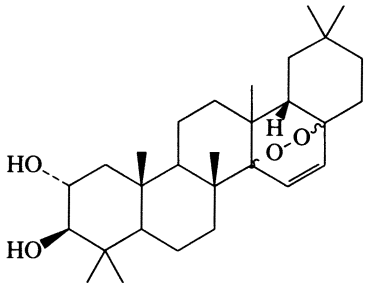
Bindl, J. *et al*, *Chem. Ber.*, 1983, **116**, 2408 (*synth, uv, pmr*)

B

Baccatin **B-80001**

Updated Entry replacing B-00002

[66107-60-6]



$C_{29}H_{46}O_4$ M 458.680

Constit. of *Sapium baccatum*. Cryst. Mp 228-229° dec. $[\alpha]_D$ −9.09°.

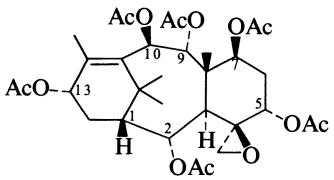
Saha, B. *et al*, *Tetrahedron Lett.*, 1977, 3095.

Baccatin I **B-80002**

Updated Entry replacing B-00003

2α,5α,7β,9α,10β,13α-Hexaacetoxy-4β,20-epoxy-11-taxene

[30244-35-0]



$C_{32}H_{44}O_{13}$ M 636.692

Constit. of *Taxus baccata*. Cryst. Mp 298°. $[\alpha]_D$ +86°.

5-Deacetyl: [30244-36-1].

$C_{30}H_{42}O_{12}$ M 594.655

Constit. of *T. baccata*. Cryst. Mp 256-258°.

1β-Hydroxy: [30244-37-2]. ***1β-Hydroxybaccatin I***

$C_{32}H_{44}O_{14}$ M 652.691

Constit. of *T. baccata*. Cryst. Mp 273°. $[\alpha]_D$ +102°.

1β-Acetoxy, 5-deacetyl: [119120-27-3]. ***1β-Acetoxy-5-deacetylbaccatin I.*** *1β,2α,7β,9α,10β,13α-Hexaacetoxy-4β,20-epoxy-11-taxen-5α-ol*

$C_{32}H_{44}O_{14}$ M 652.691

Constit. of *T. mairei*. Cryst. (EtOH). Mp 240-241°.

de Marcano, D.P.D.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 1381 (*isol, struct*)

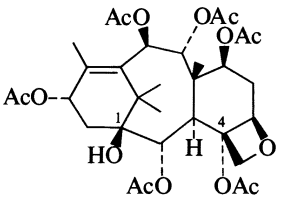
Lian, J.-Y. *et al*, *Phytochemistry*, 1988, **27**, 3674 (*deriv*)

Baccatin IV **B-80003**

Updated Entry replacing B-30001

2α,4α,7β,9α,10β,13α-Hexaacetoxy-5β,20-epoxy-11-taxen-1β-ol

[57672-77-2]



$C_{32}H_{44}O_{14}$ M 652.691

Constit. of *Taxus baccata*. Cryst. Mp 254-255° dec. $[\alpha]_D$ +19°.

1-Deoxy, 4-deacetyl: [119120-26-2]. ***1-Dehydroxy-4-deacetylbaccatin IV.*** *2α,7β,9α,10β,13α-Pentaacetoxy-5β,20-epoxy-11-taxen-4α-ol*

$C_{30}H_{42}O_{12}$ M 594.655

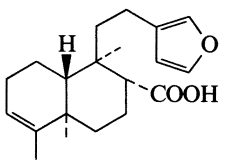
Constit. of *T. mairei*. Cryst. (EtOH). Mp 229-230°. $[\alpha]_D^{14}$ +40° (c, 0.5 in Me_2CO).

de Marcano, D.P.D.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 365 (*isol, struct*)

McLaughlin, J.L. *et al*, *J. Nat. Prod.* (*Lloydia*), 1981, **44**, 312 (*isol*)

Lian, J.-Y. *et al*, *Phytochemistry*, 1988, **27**, 3674 (*deriv*)

Bacchabolivic acid **B-80004**



$C_{20}H_{28}O_3$ M 316.439

Constit. of *Baccharis boliviensis*. Cryst. Mp 147°.

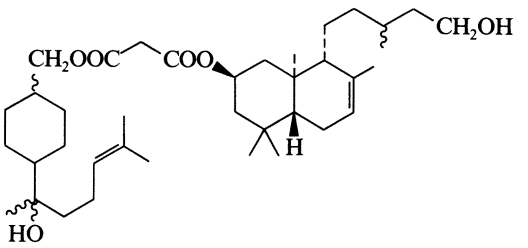
Xylopyranoside:

$C_{25}H_{36}O_7$ M 448.555

Constit. of *B. boliviensis*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

Bacchalatifolin **B-80005**



$C_{38}H_{64}O_6$ M 616.920

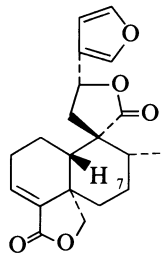
Constit. of *Baccharis latifolia*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

Bacchotricuneatin B B-80006

Updated Entry replacing B-00016

[65596-26-1]



$C_{20}H_{22}O_5$ M 342.391

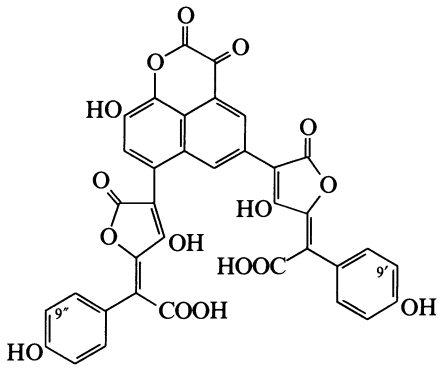
Constit. of *Baccharis tricuneata*. Cryst. (CH_2Cl_2/hexane). Mp 192-193°. $[\alpha]_D^{25}$ −102.4° (c, 0.55 in $CHCl_3$).

7α-Acetoxy: [116139-48-1]. ***7α-Acetoxybacchotricuneatin B***
$C_{22}H_{24}O_7$ M 400.427
Constit. of *Olearia pimeleoides*. Gum.

Wagner, H. *et al*, *Tetrahedron Lett.*, 1977, 3039 (*isol, struct*)
Warning, U. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 513 (*deriv*)

Badione A B-80007

[90295-66-2]



$C_{36}H_{18}O_{16}$ M 706.529

Pigment from the bay boletus *Xerocomus badius* and from *Boletus pinicola*. Shiny blackish-brown microcryst. Dec. >250° without melting. λ_{max} 260, 368, 482sh nm.

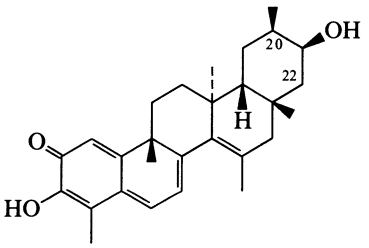
9′,9″-Dihydroxy: [97486-15-2]. ***Badione B***
$C_{36}H_{18}O_{18}$ M 738.527
Pigment from *B. erythropus*.

Steffan, B. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 445 (*isol, cmr, struct*)

Balaenol B-80008

Updated Entry replacing B-70006

[115031-67-9]



$C_{28}H_{36}O_3$ M 420.591

Constit. of *Cassine balae*. Mp 139-140°.

22-Oxo: [115028-52-9]. ***Balaenonol***
$C_{28}H_{34}O_4$ M 434.574
Constit. of *C. balae*. Mp 205-208°.

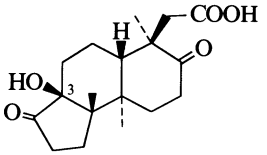
20-epimer,22β-hyddroxy: ***Isobalaendiol***
$C_{28}H_{36}O_4$ M 436.590
Constit. of *C. balae*. Orange-red solid (CH_2Cl_2/Et_2O). Mp 210-213°. $[\alpha]_D$ +65° (c, 4.5 in $CHCl_3$).

Fernando, H.C. *et al*, *Tetrahedron Lett.*, 1988, **29**, 387 (*struct*)
Fernando, H.C. *et al*, *Tetrahedron*, 1989, **45**, 5867 (*Isobalaendiol*)

Barbacenic acid B-80009

Updated Entry replacing B-40004

[97746-05-9]



$C_{18}H_{26}O_5$ M 322.400

Constit. of *Barbacenia flava*.

Me ester: Cryst. Mp 137-139°. $[\alpha]_D^{25}$ +40° (c, 0.6 in $CHCl_3$).

3-Deoxy: [119967-64-5]. ***3-Deoxybarbacenic acid***
$C_{18}H_{26}O_4$ M 306.401
Constit. of *B. flava*. Cryst. (EtOAc/hexane). Mp 200-202°.

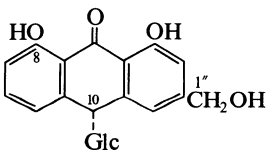
Pinto, A.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 446 (*isol*)
Pinto, A.C. *et al*, *Phytochemistry*, 1988, **27**, 3917 (*3-Deoxybarbacenic acid*)

Barbaloin B-80010

Updated Entry replacing B-00074

10-β-D-Glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10H)-anthracenone, 9CI. Aloin. Socaloin. Ugandaloin. Jafaloin. Cafaloin

[1415-73-2]



(10*R*)-*form*

$C_{21}H_{22}O_9$ M 418.399

Found in Barbados aloes. Yellow needles (EtOH). Sol. H_2O. Mp 150°, Mp 146-148°. $[\alpha]_D$ −8.3° (EtOH aq.), $[\alpha]_D$ −10.4° (EtOAc). The 10-config. is as given in CA but does not appear to be clearly stated in the lit.

▷ LZ6520000.

Ac: Cryst. (pet. ether). Mp 95-96°.

Hepta-Me ether: [13954-21-7].
Prisms (EtOH). Mp 177-179°. $[\alpha]_{46}$ −12.05° ($CHCl_3$).

10-Epimer: [28371-16-6]. ***Isobarbaloin***
$C_{21}H_{22}O_9$ M 418.399
Present in *A.* spp. Yellow needles (H_2O). $[\alpha]_D$ −19.4° (EtOAc).

1″-O-α-L-Rhamnopyranosyl: [11006-91-0]. ***Aloinoside B***
$C_{27}H_{32}O_{13}$ M 564.542
Isol. from *Aloe* cf. *perryi*. Cryst. (Me_2CO aq.). Mp 233°. $[\alpha]_D^{20}$ −45.3° (c, 1.5 in 50% dioxan aq.).

8-β-D-Glucoside (stereoisomer 1): [53823-08-8]. ***Cascaroside A***
$C_{27}H_{32}O_{14}$ M 580.541

Constit. of *Rhamnus purshiana* (*Cascarae sagradae*). Cryst. + $2H_2O$. Mp 184-187°. $[\alpha]_D^{30}$ +36.8° (MeOH). Cascarosides *A* and *B* are a pair of 10-epimers (config. unknown) which equilibrate *via* the anthranol tautomer in Py/DMSO soln.

8-β-D-Glucoside (stereoisomer 2): ***Cascaroside B***
$C_{27}H_{32}O_{14}$ M 580.541
From *R. purshianus*. Cryst. + $2H_2O$. Mp 175-178°. $[\alpha]_D^{30}$ −104.4° (MeOH).

1′-Deoxy, 8-β-D-Glucoside(stereoisomer 1): ***Cascaroside C***
$C_{27}H_{32}O_{13}$ M 564.542
From *R. purshiana*. Cascarosides C and D are a pair of epimers resembling Cascarosides A and B.

1′-Deoxy, 8-β-D-Glucoside(stereoisomer 2): [53861-35-1]. ***Cascaroside D***
$C_{27}H_{32}O_{13}$ M 564.542
From *R. purshiana*.

1″-O-α-L-Rhamnopyranesyl: ***Aloinoside B***
$C_{27}H_{32}O_{13}$ M 564.542
Isol. from *Aloe* cf. *perryi*. Cryst. (Me_2CO aq.). Mp 233°. $[\alpha]_D^{20}$ −45.3° (c, 1.5 in 50% dioxan aq.).

Owen, L. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 2516 (*struct*)
Mühlemann, H., *Pharm. Acta Helv.*, 1952, **27**, 17 (*struct*)
Böhme, H. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1955, **286**, 510 (*synth*)
Birch, A.J. *et al*, *Aust. J. Chem.*, 1955, **8**, 523 (*struct*)
Hay, J.E. *et al*, *J. Chem. Soc.*, 1956, 3141 (*struct*)
Hörhammer, L. *et al*, *Z. Naturforsch.*, *B*, 1964, **19**, 222 (*Aloinoside B*)
van Oudtshoorn, M.C.Bvan.R. *et al*, *Naturwissenschaften*, 1965, **52**, 186 (*occur*)
Piox, A., *Tetrahedron*, 1968, **24**, 3697 (*ms*)
Wagner, H. *et al*, *Z. Naturforsch.*, *C*, 1974, **29**, 444; *Z. Naturforsch.*, *B*, 1976, **31**, 267 (*Cascarosides*)
Auterhoff, H. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1980, **313**, 113 (*resoln*)
Martindale, *The Extra Pharmacopoeia*, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 7502.
Rauwald, H.W. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1984, **317**, 362 (*pmr*)

Benz[*a*]anthracen-10-o1, 9CI — B-80011

10-Hydroxybenz[a]*anthracene*
[69884-53-3]
$C_{18}H_{12}O$ M 244.292
Pale yellow cryst. (C_6H_6). Mp 219-221°.

O-Benzoyl: [71685-67-1].
$C_{25}H_{16}O_2$ M 348.400
Pale yellow needles (C_6H_6/hexane). Mp 174-176°.

Fu, P.P. *et al*, *J. Org. Chem.*, 1979, **44**, 4265 (*synth, deriv, pmr*)
Pataki, J. *et al*, *J. Org. Chem.*, 1989, **54**, 840 (*synth*)

Benz[*a*]anthracen-11-o1, 9CI — B-80012

11-Hydroxybenz[a]*anthracene*
[63019-35-2]
$C_{18}H_{12}O$ M 244.292
Cryst. (C_6H_6/hexane). Mp 120-124°.

O-Ac: [71685-69-3].
$C_{20}H_{14}O_2$ M 286.329
Cryst. (C_6H_6/hexane). Mp 121-124°.

Fu, P.P. *et al*, *J. Org. Chem.*, 1979, **44**, 4265 (*synth, deriv, pmr*)

Benzenecarbodithioic acid anhydrosulfide, 9CI — B-80013

Bis(dithiobenzoic) thioanhydride
[22778-02-5]

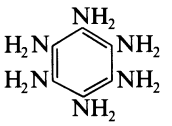
PhCS-S-CSPh

$C_{14}H_{10}S_3$ M 274.431
Dark blue oil.

Kato, S. *et al*, *Justus Liebigs Ann. Chem.*, 1982, 1229 (*synth, ir, uv, nmr*)
Kato, S. *et al*, *Synthesis*, 1987, 304 (*synth, uv, pmr, cmr, ms*)

Benzenehexamine, 9CI — B-80014

Updated Entry replacing B-60012
Hexaaminobenzene
[4444-26-2]



$C_6H_{12}N_6$ M 168.201
Needles. Mp ca. 255°. Formerly descr. as a dark-brown cryst. powder. Prepn. under Ar is necessary to obt. a colourless prod. V. air- and light-sensitive.

▷ Potentially hazardous synth.

$N^1,N^1,N^2,N^2,N^3,N^3,N^4,N^4,N^5,N^5$-*Deca-Me:* [114422-56-9]. *Pentakis(dimethylamino)aniline*
$C_{16}H_{32}N_6$ M 308.469
Cryst. solid (Me_2CO). Mp 171-172°.

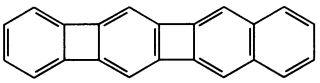
N-*Dodeca-Me:* [114396-17-7]. *Hexakis(dimethylamino)benzene*
$C_{18}H_{36}N_6$ M 336.523
Cryst. solid (Me_2CO). Mp 235-237°.

N-*Dodeca-Et:* [114396-23-5]. *Hexakis(diethylamino)benzene*
$C_{30}H_{60}N_6$ M 504.844
Cryst. (Me_2CO). Mp 211-213°.

Kohne, B. *et al*, *Justus Liebigs Ann. Chem.*, 1987, 265 (*synth, ir, pmr, cmr, ms*)
Chance, J.M. *et al*, *J. Org. Chem.*, 1988, **53**, 3226 (*derivs, synth, pmr, cmr, cryst struct*)

Benzo[*b*]benzo[3,4]cyclobuta[1,2-*h*] biphenylene, 9CI — B-80015

*Naphtho[2′,3′:3,4]cyclobuta[1,2-*b*]biphenylene*
[117965-75-0]

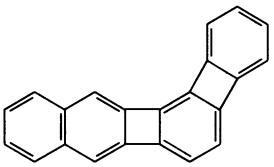


$C_{22}H_{12}$ M 276.337
Bright orange microcryst. Highly insol. Mp >305° dec.(subl. >250°).

Shepherd, M.K., *J. Chem. Soc., Perkin Trans.* 1, 1988, 961 (*synth, ms, pmr*)

Benzo[*h*]benzo[3,4]cyclobuta[1,2-*a*] biphenylene, 9CI — B-80016

*Naphtho[2′,3′:3,4]cyclobuta[1,2-*a*]biphenylene*
[117965-76-1]



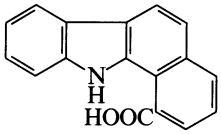
$C_{22}H_{12}$ M 276.337

Lemon yellow cryst. Mp 192-194° (subl. >145°). Blue fluor. in dil. soln.

Shepherd, M.K., *J. Chem. Soc., Perkin Trans.* 1, 1988, 961 (*synth, pmr, cmr, ms*)

11*H*-Benzo[*a*]carbazole-1-carboxylic acid B-80017

[93328-83-7]



$C_{17}H_{11}NO_2$ M 261.279
Cryst. ($CHCl_3$). Mp 230-232°.

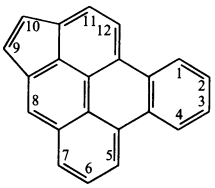
Me ester:
$C_{18}H_{13}NO_2$ M 275.306
Light yellow needles (MeOH). Mp 99.5-100.6°.

Dokunikhin, N.S. *et al, J. Gen. Chem. USSR* (*Engl. Transl.*), 1963, **33**, 962 (*synth*)
Katritzky, A.R. *et al, J. Org. Chem.*, 1988, **53**, 794 (*synth, pmr*)

Benzo[*l*]cyclopenta[*cd*]pyrene, 9CI B-80018

Naphth[*1,2,3*-mno]*acephenanthrylene*

[113779-16-1]

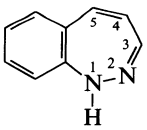


$C_{22}H_{12}$ M 276.337
Yellow-orange solid. Mp 190-191°.

Sangaiah, R. *et al, J. Org. Chem.*, 1988, **53**, 2620 (*synth, pmr, ir, uv, ms*)

1*H*-1,2-Benzodiazepine, 9CI B-80019

[264-60-8]



$C_9H_8N_2$ M 144.176
Red prisms (diisopropyl ether). Mp 63-64°.

Tsuchiya, T. *et al, J. Org. Chem.*, 1977, **42**, 1856 (*synth, ir, ms, pmr*)

3*H*-1,2-Benzodiazepine, 9CI B-80020

[55379-61-8]

Yellow oil. Bp_1 126-128° (bath) .

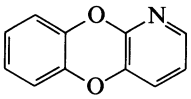
1-Oxide: [59066-30-7].
$C_9H_8N_2O$ M 160.175
Prisms (C_6H_6/diisopropyl ether). Mp 93-94°.

2-Oxide: [59066-32-9].
$C_9H_8N_2O$ M 160.175
Prisms (C_6H_6/diisopropyl ether). Mp 85-86°.

Tsuchiya, T. *et al, Chem. Pharm. Bull.*, 1978, **26**, 1890, 1896 (*synth, pmr, uv, oxides*)

[1,4]Benzodioxino[2,3-*b*]pyridine B-80021

[72850-33-0]



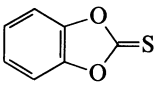
$C_{11}H_7NO_2$ M 185.182
Greyish solid. Mp 95-97°.

Sutherland, R.G. *et al, J. Heterocycl. Chem.*, 1988, **25**, 1911 (*synth, pmr, cmr*)

1,3-Benzodioxole-2-thione, 9CI B-80022

Thiocarbonic acid cyclic O,O-*o-phenylene ester, 8CI. 2-Thioxobenzodioxole*

[2231-05-2]

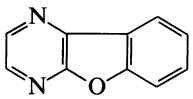


$C_7H_4O_2S$ M 152.173
Pale-pink needles (EtOH). Mp 152-153°.

Autenreith, A. *et al, Ber.*, 1925, **58**, 2151 (*synth*)
Sugimoto, H. *et al, J. Org. Chem.*, 1988, **53**, 2263 (*synth*)

Benzofuro[2,3-*b*]pyrazine, 9CI B-80023

[114954-31-3]



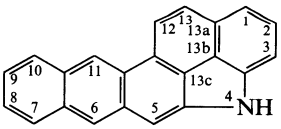
$C_{10}H_6N_2O$ M 170.170
Needles. Mp 89-90°.

Taylor, E.C. *et al, Tetrahedron*, 1987, **43**, 5159 (*synth, ir, pmr*)

4*H*-Benzo[*def*]naphtho[2,3-*b*]carbazole, 9CI B-80024

4,5-Iminobenzo[k]*chrysene. Naphtho*[*2′,3′:1,2*]-*4,5-iminophenanthrene* (incorr.)

[42130-22-3]



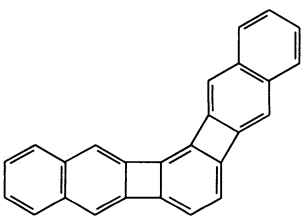
$C_{22}H_{13}N$ M 291.351
Reg. no. refers to 1*H*-form. Yellow plates (xylene). Mp 379-380°.

Zander, M. *et al, Chem. Ber.*, 1966, **99**, 1279 (*synth, uv*)

Benzo[*h*]naphtho[2′,3′:3,4]cyclobuta[1,2-*a*] biphenylene, 9CI B-80025

Benzo[*1‴,2‴:3,4:3″,4″:3′,4′*]*dicyclobuta*[*1,2*-b*:1′,2′*-b′]*dinaphthalene*

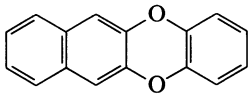
[117965-77-2]



$C_{26}H_{14}$ M 326.397
Pale yellow cryst. by subl. Mp 295-298° (subl. >200°). Greenish fluor. in dil. soln.

Shepherd, M.K., *J. Chem. Soc., Perkin Trans.* 1, 1988, 961 (*synth, pmr, ms*)

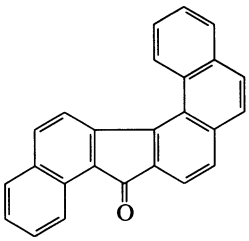
Benzo[*b*]naphtho[2,3-*e*][1,4]dioxan **B-80026**
5,12-Dioxanaphthacene



$C_{16}H_{10}O_2$ M 234.254
Silvery microcryst. Mp 202-203°.

Sutherland, R.G. *et al, J. Heterocycl. Chem.*, 1988, **25**, 1911 (*synth, pmr, cmr*)

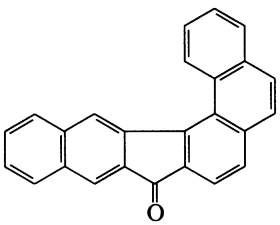
Benzo[*a*]naphtho[2,1-*d*]fluoren-9-one **B-80027**
[114469-09-9]



$C_{25}H_{14}O$ M 330.385
Yellow solid. Mp 244-245° (238-239°).

Campbell, A.D., *J. Chem. Soc.*, 1954, 3659 (*synth*)
Smith, J.G. *et al, J. Org. Chem.*, 1988, **53**, 2942 (*synth, pmr*)

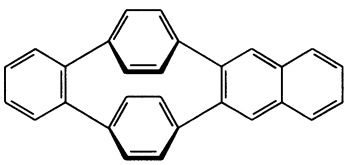
Benzo[*b*]naphtho[2,1-*d*]fluoren-9-one **B-80028**
[114469-08-8]



$C_{25}H_{14}O$ M 330.385
Red solid. Mp 203-204° (193-195°).

Campbell, A.D., *J. Chem. Soc.*, 1954, 3659 (*synth*)
Smith, J.G. *et al, J. Org. Chem.*, 1988, **53**, 2942 (*synth, pmr*)

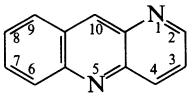
Benzonaphtho[2.2]paracyclophane **B-80029**
*6,9:14,17-Diethenobenzo[7,8]cyclododeca[1,2-*b*]naphthalene, 9CI*
[97315-27-0]



$C_{28}H_{18}$ M 354.450
Cryst. (toluene). Mp 278° dec.

Chan, C.W. *et al, J. Am. Chem. Soc.*, 1988, **110**, 462 (*synth, uv, pmr*)

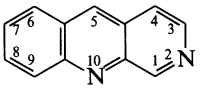
Benzo[*b*]-[1,5]-naphthyridine **B-80030**
1,10-Diaazaanthracene
[261-05-2]



$C_{12}H_8N_2$ M 180.209
Cryst. Mp 106-107°. $Bp_{0.08}$ 65° subl.

Hicks, M.G. *et al, J. Chem. Soc., Perkin Trans.* 1, 1988, 69 (*synth, uv, pmr*)

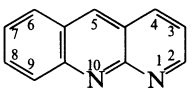
Benzo[*b*][1,7]naphthyridine **B-80031**
2,9-Diazaanthracene
[260-95-7]



$C_{12}H_8N_2$ M 180.209
Cryst. (cyclohexane). Mp 134-135°. $Bp_{0.02}$ 60°.

Hicks, M.G. *et al, J. Chem. Soc., Perkin Trans.* 1, 1988, 69 (*synth, uv, pmr, ms*)

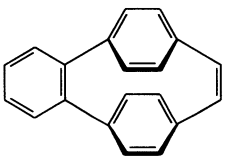
Benzo[*b*][1,8]naphthyridine **B-80032**
1,9-Diaazaanthracene
[261-00-7]



$C_{12}H_8N_2$ M 180.209
Mp 190-192°.

Hamada, Y. *et al, Chem. Pharm. Bull.*, 1974, **22**, 485.
Hicks, M.G. *et al, J. Chem. Soc., Perkin Trans.* 1, 1988, 69 (*synth*)

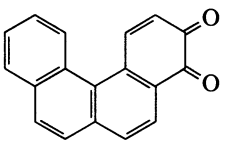
Benzo[2.2]paracyclophan-9-ene **B-80033**
5,8:11,14-Diethenobenzocyclododecene, 9CI
[64586-11-4]



$C_{20}H_{14}$ M 254.331
Platelets (heptane). Mp 227-229°.

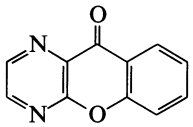
Jacobson, N. *et al, Angew. Chem., Int. Ed. Engl.*, 1978, **17**, 46 (*synth, pmr*)
Chan, C.W. *et al, J. Am. Chem. Soc.*, 1988, **110**, 462 (*synth, uv, pmr*)

Benzo[*c*]phenanthrene-3,4-dione **B-80034**
Benzo[c]*phenanthrene-3,4-quinone*
[118658-88-1]



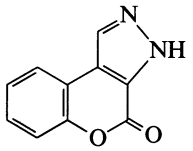
$C_{18}H_{10}O_2$ M 258.276
Cryst. (C_6H_6). Mp 178-180°.
Pataki, J. *et al*, *J. Org. Chem.*, 1989, **54**, 840 (*synth*, *pmr*)

10*H*-[1]Benzopyrano[2,3-*b*]pyrazin-10-one, 9CI **B-80035**
1,4-Diazaxanthone
[121246-97-7]



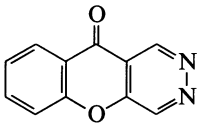
$C_{11}H_6N_2O_2$ M 198.181
Cryst. Mp 224°.
Turck, A. *et al*, *Synthesis*, 1988, 881 (*synth*, *pmr*)

[1]Benzopyrano[3,4-*c*]pyrazol-4(3*H*)-one, 9CI **B-80036**
[91166-74-4]



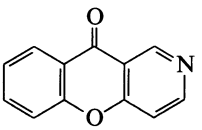
$C_{10}H_6N_2O_2$ M 186.170
Needles (dioxan). Mp >250°.
Ito, K. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1681 (*synth*, *pmr*)

10*H*-[1]Benzopyrano[2,3-*d*]pyridazin-10-one, 9CI **B-80037**
[115276-46-5]



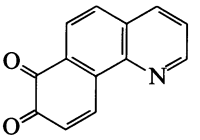
$C_{11}H_6N_2O_2$ M 198.181
Pale yellow cryst. (MeOH). Mp 189-190°.
Haider, N. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1988, 401 (*synth*, *ir*, *pmr*, *ms*)

10*H*-[1]Benzopyrano[3,2-*c*]pyridin-10-one, 9CI **B-80038**
2-Azaxanthone
[54629-30-0]



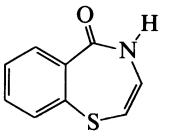
$C_{12}H_7NO_2$ M 197.193
Cryst. (C_6H_6/pet. ether). Mp 185°.
Ghosh, C.K. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1988, 1489 (*synth*, *ir*, *uv*, *pmr*, *ms*)

Benzo[*h*]quinoline-7,8-dione **B-80039**
[113163-25-0]



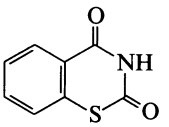
$C_{13}H_7NO_2$ M 209.204
Dark red solid (C_6H_6). Mp 118°.
Czech, A. *et al*, *J. Org. Chem.*, 1988, **53**, 1329 (*synth*, *ms*, *pmr*)

1,4-Benzothiazepin-5(4*H*)-one **B-80040**
[115483-67-5]



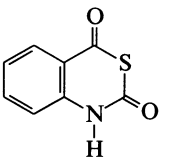
C_9H_7NOS M 177.226
Cryst. (MeOH). Mp 143.5-145°.
N-*Me:* [115483-68-6].
$C_{10}H_9NOS$ M 191.253
Orange-tinted cryst. (MeOH). Mp 84-84.5°.
Hofmann, H. *et al*, *Chem. Ber.*, 1988, **121**, 2147 (*synth*, *pmr*)

2*H*-1,3-Benzothiazine-2,4(3*H*)-dione **B-80041**
[10512-65-9]



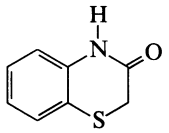
$C_8H_5NO_2S$ M 179.199
Cryst. (EtOH). Mp 216°.
Palazzo, S. *et al*, *Gazz. Chim. Ital.*, 1963, **93**, 207 (*synth*)

2*H*-3,1-Benzothiazine-2,4(1*H*)-dione **B-80042**
[703-65-1]



$C_8H_5NO_2S$ M 179.199
Cryst. (EtOAc). Mp 232-233° (226-235°).
N-*Me:*
$C_9H_7NO_2S$ M 193.226
Fine prisms (EtOH or Me_2CO). Mp 170.5-172°.
Marshall, J.R., *J. Chem. Soc.*, 1965, 938 (*synth*)
Kricheldorf, H.R., *Chem. Ber.*, 1971, **104**, 3156 (*ir*)
Sugimoto, H. *et al*, *J. Org. Chem.*, 1988, **53**, 2263 (*synth*)

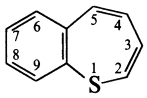
2*H*-1,4-Benzothiazin-3(4*H*)-one, 9CI **B-80043**
*3,4-Dihydro-3-oxo-2*H*-1,4-benzothiazine*
[5325-20-2]



C_8H_7NOS M 165.215
Cryst. (DMF/MeCN). Mp 177-179°.
N-Me: [37142-87-3].
C_9H_9NOS M 179.242
Cryst. Mp 50-53°.

Krapcho, J. *et al*, *J. Med. Chem.*, 1973, **16**, 776 (*synth*)
Worley, J.W. *et al*, *J. Org. Chem.*, 1975, **40**, 1731 (*deriv*, *synth*, *pmr*)

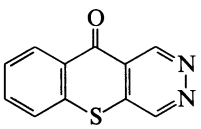
1-Benzothiepin **B-80044**
Updated Entry replacing B-00575
[264-82-4]



$C_{10}H_8S$ M 160.239
Pale-yellow needles. Mp 23.5-24.5°. λ_{max} 217 (log ϵ 4.07), 256(4.07), 295 sh (2.96) and 345 nm (2.55)(cyclohexane).
1-Oxide:
$C_{10}H_8OS$ M 176.239
Pale-yelow needles at −40°. Dec. to naphthalene after 1h at 13°.
1,1-Dioxide: [41887-86-9].
$C_{10}H_8O_2S$ M 192.238
Mp 138-139°.

Traynelis, V.J. *et al*, *J. Org. Chem.*, 1973, **38**, 3978 (*synth*)
Murata, I. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1974, **13**, 142 (*synth*)
Yasuoka, N. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1974, **15**, 297 (*cryst struct*, *deriv*)
Nishino, K. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1988, **27**, 1717 (*oxide*)

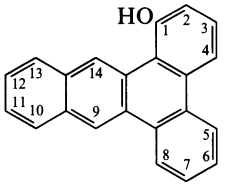
10*H*-[1]Benzothiopyrano[2,3-*d*]pyridazin-10-one, 9CI **B-80045**
[115276-47-6]



$C_{11}H_6N_2OS$ M 214.247
Pale yellow needles (Me_2CO). Mp 228-229°.

Haider, N. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1988, 401 (*synth*, *pmr*, *ir*, *ms*)

Benzo[*b*]triphenylen-1-ol, 9CI **B-80046**
1-Hydroxydibenz[a,c]*anthracene*
[115165-01-0]



$C_{22}H_{14}O$ M 294.352
Cryst. (C_6H_6). Mp 210-211°.

Kole, P.L. *et al*, *J. Org. Chem.*, 1989, **54**, 845 (*synth*, *pmr*)

Benzo[*b*]triphenylen-2-ol, 9CI **B-80047**
2-Hydroxydibenz[a,c]*anthracene*
[113058-38-1]
$C_{22}H_{14}O$ M 294.352
Cryst. (Et_2O). Mp 287-288°.

Kole, P.L. *et al*, *J. Org. Chem.*, 1989, **54**, 845 (*synth*, *pmr*)

Benzo[*b*]triphenylen-3-ol, 9CI **B-80048**
3-Hydroxydibenz[a,c]*anthracene*
[88488-97-5]
$C_{22}H_{14}O$ M 294.352
Cryst. (Et_2O). Mp 252-253°.

Harvey, R.G. *et al*, *Org. Prep. Proced. Int.*, 1983,, **15**, 335 (*synth*)
Kole, P.L. *et al*, *J. Org. Chem.*, 1989, **54**, 845 (*synth*, *pmr*)

Benzo[*b*]triphenylen-4-ol, 9CI **B-80049**
4-Hydroxydibenz[a,c]*anthracene*
[113058-39-2]
$C_{22}H_{14}O$ M 294.352
Cryst. (C_6H_6). Mp 266-267°.

Kole, P.L. *et al*, *J. Org. Chem.*, 1989, **54**, 845 (*synth*, *pmr*)

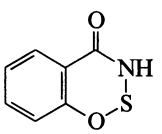
Benzo[*b*]triphenylen-10-ol, 9CI **B-80050**
10-Hydroxydibenz[a,c]*anthracene*
[39081-15-7]
$C_{22}H_{14}O$ M 294.352
Cryst. (Et_2O/hexane). Mp 239-241° (220-222°).

Sims, P., *Biochem. J.*, 1972, **130**, 27 (*synth*, *uv*)
Kole, P.L. *et al*, *J. Org. Chem.*, 1989, **54**, 845 (*synth*, *pmr*)

Benzo[*b*]triphenylen-11-ol, 9CI **B-80051**
11-Hydroxydibenz[a,c]*anthracene*
[39147-43-8]
$C_{22}H_{14}O$ M 294.352
Cryst. (C_6H_6). Mp 200-201°.

Sims, P., *Biochem. J.*, 1972, **130**, 27 (*synth*, *uv*)
Kole, P.L. *et al*, *J. Org. Chem.*, 1989, **54**, 845 (*synth*, *pmr*)

1,2,3-Benzoxathiazin-4(3*H*)-one, 9CI **B-80052**
3,4-Dihydro-4-oxo-1,2,3-benzothiazine



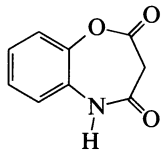
$C_7H_5NO_2S$ M 167.188
2,2-Dioxide: [51299-06-0].

$C_7H_5NO_4S$ M 199.187
Cryst. ($CHCl_3$/hexane). Mp 218-220° dec.

Kamal, A. *et al*, *J. Org. Chem.*, 1988, **53**, 4112 (*synth, ir, pmr*)

1,5-Benzoxepine-2,4-(3*H*,5*H*)-dione B-80053

[84755-33-9]



$C_9H_7NO_3$ M 177.159
Cryst. (EtOH). Mp 199-201°. A synthesis claimed in 1982 appears to be erroneous.

Bartsch, H. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 177 (*synth, pmr*)

2-Benzoylbenzoic acid, 9CI B-80054

Updated Entry replacing B-00632
Benzophenone-2-carboxylic acid. Diphenylmethanone-2-carboxylic acid
[85-52-9]

$C_{14}H_{10}O_3$ M 226.231
Needles + $1H_2O$ (H_2O), cryst. (C_6H_6/pet. ether). Mp 95° (hydrate), Mp 128° (anhyd.). pK_a 3.43.

Me ester: [606-28-0].
$C_{15}H_{12}O_3$ M 240.258
Prisms. Mp 52°. Bp 352°.

Et ester: [604-61-5].
$C_{16}H_{14}O_3$ M 254.285
Mp 58°.

Chloride: [22103-85-1].
$C_{14}H_9ClO_2$ M 244.677
Prisms. Mp 70°.

Anhydride:
$C_{28}H_{18}O_5$ M 434.447
Mp 140°.

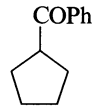
Amide: [7500-78-9].
$C_{14}H_{11}NO_2$ M 225.246
Mp 165°.

Nitrile: [37774-78-0]. o-*Cyanobenzophenone*
$C_{14}H_9NO$ M 207.231
Cryst. Mp 83-84°.

Rubidge, C.R. *et al*, *J. Am. Chem. Soc.*, 1914, **36**, 732 (*synth*)
CRC Atlas of Spectral Data and Physical Constants, 1962 (*ir, uv, ms, nmr*)
Delettre, J., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1969, **269**, 113 (*cryst struct*)
Vogel, A.I., *Textbook of Practical Organic Chemistry*, Longman, London, 4th Ed., 1978, 780 (*synth*)
Ebert, G.W. *et al*, *J. Org. Chem.*, 1988, **53**, 4482 (*nitrile*)

Benzoylcyclopentane B-80055

Cyclopentylphenylmethanone, 9CI. Cyclopentyl phenyl ketone
[5422-88-8]



$C_{12}H_{14}O$ M 174.242
Oil. Bp_{16} 138-140°, $Bp_{0.05}$ 89-90°. n_D^{20} 1.5290, 1.5404.

Oxime: [83568-09-6].
$C_{12}H_{15}NO$ M 189.257
Needles (pet. ether). Mp 106-108°.

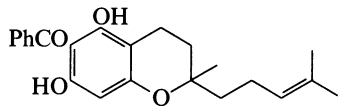
Semicarbazone: Needles (C_6H_6). Mp 107.5-109.5°.

2,4-Dinitrophenylhydrazone: Yellow cryst. (EtOH). Mp 142-143°.

Hey, D.H. *et al*, *J. Chem. Soc.*, 1949, 3156 (*synth*)
Zhang, P. *et al*, *Synth. Commun.*, 1986, **16**, 957 (*synth*)

6-Benzoyl-5,7-dihydroxy-2-methyl-2-(4-methyl-3-pentenyl)chroman B-80056

3,4-Dihydro-5,7-dihydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2H-benzopyran-6-ylphenylmethanone



$C_{23}H_{26}O_4$ M 366.456
Isol. from *Helichrysum monticola*. Oil. Not abstracted by CA. Incorrectly named in the reference.

Bohlmann, F. *et al*, *Phytochemistry*, 1980, **19**, 683.

2-Benzoylpropanal B-80057

Updated Entry replacing B-00700
α-Methyl-β-oxobenzenepropanal, 9CI. 2-Benzoylpropionaldehyde, 8CI. 1-Formylethyl phenyl ketone. α-Hydroxymethylenepropiophenone. 2-Formylpropiophenone
[16837-43-7]

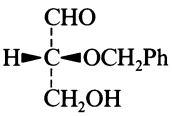
$$PhCOCH(CH_3)CHO \rightleftharpoons PhCOC(CH_3){=}CHOH$$

$C_{10}H_{10}O_2$ M 162.188
Cryst. (EtOH). Mp 118-119°.

Takagi, S. *et al*, *CA*, 1959, **53**, 18003f (*synth*)
Aspart-Pascot, L. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 483 (*synth*)

2-*O*-Benzylglyceraldehyde B-80058

3-Hydroxy-2-(phenylmethoxy)propanal, 9CI



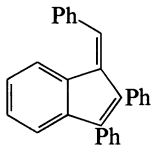
$C_{10}H_{12}O_3$ M 180.203

(R)-form [76227-09-3]
Configurationally stable chiral intermed. for synthesis. Oil with fruity odour. $[\alpha]_D$ +21.7→+16.1° (6h)→+30.3° (19d) (c, 1.23 in EtOH). Oligomerises on standing without loss of configurational homogeneity. (*S*)-enantiomer also accessible.

Jäger, V. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 469 (*synth, use*)

1-Benzylidene-2,3-diphenylindene B-80059

*2,3-Diphenyl-1-(phenylmethylene)-1*H*-indene, 9CI*



$C_{28}H_{20}$ M 356.466

(E)-form [121638-18-4]

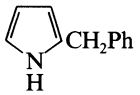
Unexpected prod. of reacn. of hexaphenylstannole with Br_2. Cryst. Mp 176°.

Muchmore, C.R.A. *et al*, *Acta Crystallogr., Sect. C*, 1989, **45**, 824 (*cryst struct*)

2-Benzylpyrrole B-80060

*2-(Phenylmethyl)-1*H*-pyrrole, 9CI*

[33234-48-9]



$C_{11}H_{11}N$ M 157.215

$Bp_{2.5}$ 130°, $Bp_{0.12\text{-}0.15}$ 85-89°.

Gogan, N.J. *et al*, *J. Organomet. Chem.*, 1972, **39**, 129 (*synth*)

McGillivray, G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1983, 633 (*synth*)

3-Benzylpyrrole B-80061

*3-(Phenylmethyl)-1*H*-pyrrole, 9CI*

[33234-57-0]

$C_{11}H_{11}N$ M 157.215

No phys. props. reported.

Groves, J.K. *et al*, *Can. J. Chem.*, 1971, **49**, 2427 (*synth, pmr, ms*)

Benzyl vinyl sulfide, 8CI B-80062

[(Ethenylthio)methyl]benzene, 9CI

[1822-76-0]

$$PhCH_2SCH{=}CH_2$$

$C_9H_{10}S$ M 150.244

Liq. d^{25}_{25} 1.038. Bp_{10} 98°, $Bp_{0.4}$ 52-56°. n^{25}_{D} 1.5773.

S-Oxide: [71841-84-4]. *Benzyl vinyl sulfoxide, 8CI.*
[(Ethylsulfinyl)methyl]benzene, 9CI
$C_9H_{10}OS$ M 166.243
Cryst. Mp 34-35°.

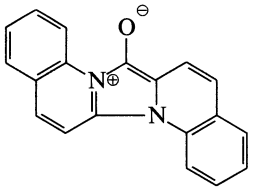
S-Dioxide: [15753-89-6]. *Benzyl vinyl sulfone, 8CI.*
[(Ethenylsulfonyl)methyl]benzene, 9CI
$C_9H_{10}O_2S$ M 182.243
Cryst.

Protiva, M., *Collect. Czech. Chem. Commun.*, 1949, **14**, 354 (*synth*)
Reppe, W. *et al*, *Justus Liebigs Ann. Chem.*, 1956, **601**, 111 (*synth*)
Schneider, H.J. *et al*, *J. Org. Chem.*, 1961, **26**, 1980 (*synth, props*)
Annunziata, R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1979, 1684 (*oxide*)
Baum, J.C. *et al*, *Can. J. Chem.*, 1984, **62**, 1687 (*synth, ir, pmr, ms*)

Besthorn's red B-80063

*14-Hydroxyimidazo[1,2-*a*: 3,4-*a*′]diquinolin-7-ium hydroxide, inner salt, 9CI*

[98779-77-2]

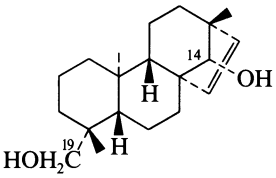


$C_{19}H_{12}N_2O$ M 284.317

Dark red glistening cryst. Mp 280° dec. (sinters from 230°). Forms MeOH solvates.

Besthorn, E. *et al*, *Ber.*, 1904, **37**, 1236 (*synth*)
Krollpfeiffer, F. *et al*, *Justus Liebigs Ann. Chem.*, 1937, **530**, 34 (*synth, uv*)
Edward, J.T. *et al*, *J. Org. Chem.*, 1985, **50**, 4855 (*synth, ir, bibl*)

ent-15-Beyerene-14β,19-diol B-80064



$C_{20}H_{32}O_2$ M 304.472

*14-*O*-Tigloyl:* ***Elasclepiol***
$C_{25}H_{38}O_3$ M 386.573
Constit. of *Elaeoselinium asclepium*. Needles (hexane). Mp 142-143°. $[\alpha]_D$ +45.4° (c, 1 in $CHCl_3$).

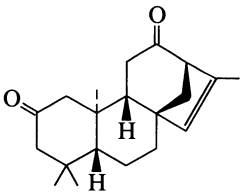
*19-Carboxylic acid, 14-*O*-tigloyl:* ***Elasclepic acid***
$C_{25}H_{36}O_4$ M 400.557
Constit. of *E. asclepium*. Oil. $[\alpha]_D$ −8.4° (c, 1.6 in EtOH).

Grande, M. *et al*, *Phytochemistry*, 1989, **28**, 1955.

ent-15-Beyerene-2,12-dione B-80065

Yucalexin B-7

[64657-12-1]

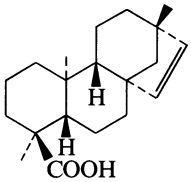


$C_{20}H_{28}O_2$ M 300.440

Constit. of cassava roots (*Manihot esculenta*).

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

ent-15-Beyeren-18-oic acid B-80066



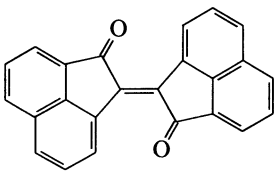
$C_{20}H_{30}O_2$ M 302.456
Constit. of *Helipterum floribundum*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 517.

1,1′-Biacenaphthylidene-2,2′-dione B-80067

2-(2-Oxo-1(2H)-acenaphthalenylidene)-1(2H)-acenaphthylenone, 9CI. $\Delta^{1,1'}$-[Biacenaphthene]-2,2′-dione, 8CI. Biacenedione

[13286-14-1]



(*E*)-*form*

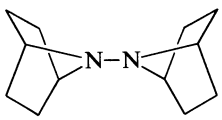
$C_{24}H_{12}O_2$ M 332.358

(*E*)-*form* [24141-18-2]
Red cryst. Mp 300° (289-291°). Most refs. do not specify the *E*-form but that is to be assumed.

Dziewonski, K. *et al*, *Chem. Ber.*, 1925, **58**, 2539 (*synth*)
Rule, H.G. *et al*, *J. Chem. Soc.*, 1937, 1761 (*synth*)
De Jong, D.C. *et al*, *Tetrahedron*, 1972, **28**, 3603 (*synth*)
Huang, N.Z. *et al*, *J. Org. Chem.*, 1987, **52**, 169 (*synth*)

7,7′-Bi-7-azabicyclo[2.2.1]heptane, 9CI B-80068

[116005-44-8]



$C_{12}H_{20}N_2$ M 192.303
Cryst. by subl. Mp 111.5-112°.

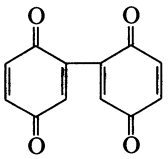
[116005-46-0]

Nelsen, S.F. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6149 (*synth, pmr, cmr*)

2,2-Bi(1,4-benzoquinone) B-80069

[Bi-1,4-cyclohexadien-1-yl]-3,3′,6,6′-tetrone, 9CI

[23783-80-4]



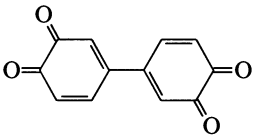
$C_{12}H_6O_4$ M 214.177
Chestnut cryst. (nitrobenzene). Mp 230°.

Paraskevas, S.M. *et al*, *Synthesis*, 1988, 897 (*synth, ir, pmr*)

4,4′-Bi(1,2-benzoquinone) B-80070

[Bi-1,5-cyclohexadien-1-yl]-3,3′,4,4′-tetrone, 9CI

[120811-93-0]



$C_{12}H_6O_4$ M 214.177
Red cryst. Mp 136° dec.

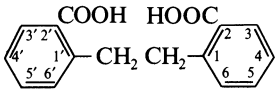
Paraskevas, S.M. *et al*, *Synthesis*, 1988, 897 (*synth, ir, pmr*)

Bibenzyl-2,2′-dicarboxylic acid B-80071

Updated Entry replacing B-00989

2,2′-(1,2-Ethanediyl)bisbenzoic acid, 9CI. α,α′-Bi-o-toluic acid, 8CI. 1,2-Bis(2-carboxyphenyl)ethane. Ethylenedibenzoic acid (misleading)

[4281-17-8]



$C_{16}H_{14}O_4$ M 270.284
Needles (EtOH), cryst. ($CHCl_3$/MeOH). Mp 237-239° (226-228°).

Di-Me ester:
$C_{18}H_{18}O_4$ M 298.338
Mp 100-101°.

Di-Et ester:
$C_{20}H_{22}O_4$ M 326.391
Needles (MeOH). Mp 67-68°.

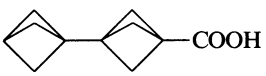
Dichloride:
$C_{16}H_{12}Cl_2O_2$ M 307.175
Liq.

Dinitrile: 2,2′-Dicyanobibenzyl
$C_{16}H_{12}N_2O_2$ M 264.283
Mp 139°.

Fuson, R.C., *J. Am. Chem. Soc.*, 1926, **48**, 830 (*synth*)
Hannemann, K. *et al*, *Helv. Chim. Acta*, 1988, **71**, 1841 (*synth, ir, pmr*)

1,1′-Bi(bicyclo[1.1.1]pentane)-3-carboxylic acid B-80072

[2]Staffane-3-carboxylic acid

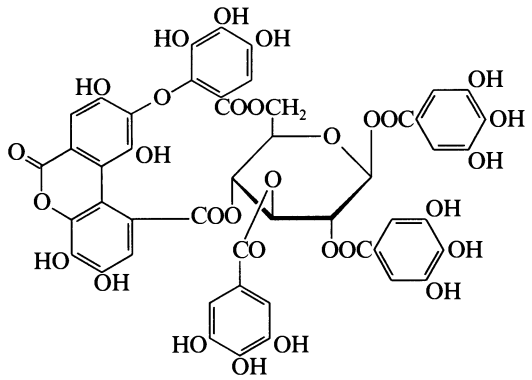


$C_{11}H_{14}O_2$ M 178.230
Cryst. Mp *ca* 200°.

Me ester:
$C_{12}H_{16}O_2$ M 192.257
Cryst. Mp ~ 60°.

Kaszynski, P. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5225 (*synth, cryst struct, pmr*)

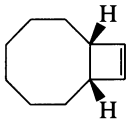
Bicornin B-80073



$C_{48}H_{32}O_{30}$ M 1088.763
Constit. of *Trapa bicornis*. Amorph. powder. $[\alpha]_D$ +4.7° (MeOH).

Yoshida, T. *et al*, *Heterocycles*, 1989, **29**, 861.

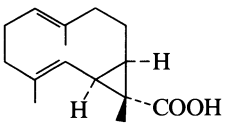
Bicyclo[6.2.0]dec-9-ene B-80074



$C_{10}H_{16}$ M 136.236
(*1RS,7SR*)-*form* [17385-24-9]
Liq.

Dauben, W.G. *et al*, *J. Org. Chem.*, 1988, **53**, 600 (*synth, ir, pmr, cmr*)

1(10),4-Bicyclogermacradien-13-oic acid B-80075

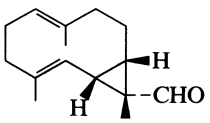


$C_{15}H_{22}O_2$ M 234.338
Constit. of *Helichrysum chionosphaerum*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

13-Bicyclogermacrenal B-80076

[118855-37-1]

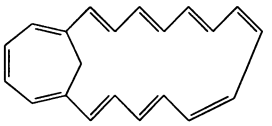


$C_{15}H_{22}O$ M 218.338
Constit. of *Conocephalum conicum*. Oil. $[\alpha]_D^{20}$ −52° (c, 0.4 in $CHCl_3$).

Toyota, M. *et al*, *Phytochemistry*, 1988, **27**, 3317.

Bicyclo[14.4.1]heneicosa-1,3,5,7,9,11,13,15,17,19-decaene, 9CI B-80077

1,6-Methano[20]annulene
[110977-29-2]

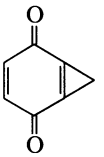


$C_{21}H_{20}$ M 272.389
Black needles (hexane). Mp 108-109°.

Yamamoto, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 395 (*synth, uv, ir, pmr*)

Bicyclo[4.1.0]hepta-1(6),3-diene-2,5-dione, 9CI B-80078

Benzocyclopropene-p-*quinone*. *Cyclopropa*-p-*benzoquinone*
[111870-65-6]

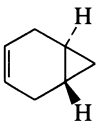


$C_7H_4O_2$ M 120.107
Unstable intermediate trapped as Diels-Alder adduct with anthracene.

Watabe, T. *et al*, *J. Org. Chem.*, 1988, **53**, 216 (*synth, ir*)

Bicyclo[4.1.0]hept-3-ene B-80079

[16554-83-9]



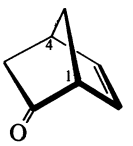
(1*RS*,6*RS*)-*form*

C_7H_{10} M 94.156
(*1RS,6RS*)-*form* [84194-54-7]
(±)-trans-*form*
Liq. Bp_{142} 45-50°.
(*1RS,6SR*)-*form* [88090-52-2]
cis-*form*
Liq. Bp 114-115°.

Simmons, H.E. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1347 (*synth*)
Plemenkov, V.V. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1974, **10**, 1672 (*synth*)
Gassman, P.G. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 667 (*synth, pmr, cmr, ir*)
Dixon, D.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2309 (*struct, bibl*)

Bicyclo[2.2.1]hept-5-en-2-one, 9CI B-80080

Updated Entry replacing B-10139
Dehydronorcamphor. *5-Norbornen-2-one*
[694-98-4]



(1*R*,4*R*)-*form*

C_7H_8O M 108.140

(1R,4R)-form [16346-63-7]
Liq. Bp_{19} 65.5-66.5°. $[\alpha]_D^{22}$ +1012° (c, 1.65 in 2,3,3-trimethylpentane)(90% e.e.).

(±)-form [51736-74-4]
Oil. Mp 22-23°. Bp_{24} 65-66.5°.

Oxime: [53838-00-9].
C_7H_9NO M 123.154
Solid (C_6H_6/EtOAc). Mp 79°.

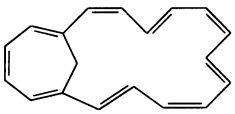
(±)-form
Oil. Mp 22-23°. Bp_{24} 65-66.5°.

Oxime:
C_7H_9NO M 123.154
Solid (C_6H_6/EtOAc). Mp 79°.

Mislow, K. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 1956 (*synth*)
Weiss, R.G. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 1172 (*synth*)
Lightner, D.A. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 5749 (*synth*)
Nakazak, N. *et al*, *J. Org. Chem.*, 1980, **45**, 4437 (*synth*)
Oppolzer, W. *et al*, *Helv. Chim. Acta*, 1985, **68**, 2100 (*synth*)
Eichberger, G. *et al*, *Tetrahedron Lett.*, 1986, **27**, 2843 (*synth*)
Mattay, J. *et al*, *Chem. Ber.*, 1989, **122**, 327 (*synth, ir, pmr, cmr*)

Bicyclo[12.4.1]nonadeca-1,3,5,7,9,11,13,15,17-nonaene B-80081

1,6-Methano[18]annulene

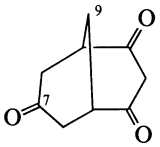


$C_{19}H_{18}$ M 246.351
Black needles (hexane). Mp 138-139°.

Yamamoto, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 395 (*synth, uv, pmr*)

Bicyclo[3.3.1]nonane-2,4,7-trione B-80082

[110935-39-2]



$C_9H_{10}O_3$ M 166.176
Needles ($CHCl_3$/hexane). Mp 158-160° (154-155°). 100% enolised in $CDCl_3$ soln. at r.t.

Hutmacher, H.-M. *et al*, *Chem. Ber.*, 1977, **110**, 3118 (*synth, nmr, ms*)
Yamazaki, T. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 3453 (*synth, pmr*)
Ebel, K. *et al*, *Chem. Ber.*, 1988, **121**, 323 (*deriv*)

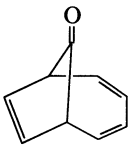
Bicyclo[3.3.1]nonane-2,4,9-trione, 9CI B-80083

[94632-45-8]
$C_9H_{10}O_3$ M 166.176
Mp 158-160°. 100% enolised in soln.

Yogev, A. *et al*, *J. Org. Chem.*, 1967, **32**, 2162.
Schoenwaelder, K.H. *et al*, *Chem. Ber.*, 1984, **117**, 3280 (*synth, pmr, cryst struct*)

Bicyclo[4.2.1]nona-2,4,7-trien-9-one, 9CI B-80084

[34733-74-9]



C_9H_8O M 132.162
Liq. solidifying on cooling. $Bp_{0.3}$ 46-47°.

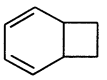
Oxime:
C_9H_9NO M 147.176
Cryst. (CH_2Cl_2/hexane). Mp 112-113°.

4-Methylbenzenesulfonylhydrazone: Solid (MeOH). Mp 177-179°.

Antkowiak, T.A. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5366 (*synth, derivs*)
Kurabayashi, K. *et al*, *Tetrahedron Lett.*, 1972, 1049 (*uv, ms*)
Diaz, A. *et al*, *J. Org. Chem.*, 1975, **40**, 2459 (*pmr*)

Bicyclo[4.2.0]octa-2,4-diene B-80085

Updated Entry replacing B-01103
[3725-28-8]

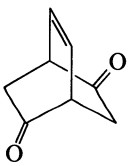


C_8H_{10} M 106.167
$Bp_{0.5}$ <30°.

Cope, A.C. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 4867 (*synth*)
Alder, K. *et al*, *Chem. Ber.*, 1954, **87**, 1492 (*synth*)
Nefedov, O.M. *et al*, *CA*, 1972, **76**, 140004y (*synth*)
Bally, C.T. *et al*, *Helv. Chim. Acta*, 1989, **72**, 73 (*synth, bibl*)

Bicyclo[2.2.2]oct-7-ene-2,5-dione B-80086

Updated Entry replacing B-50196
[17660-74-1]



(1*S*,4*S*)-*form*

$C_8H_8O_2$ M 136.150

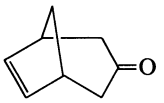
(1S,4S)-form
Cryst. Mp 98-100°. $[\alpha]_D^{29.5}$ −1257° (c, 0.0015 in cyclohexane).

(±)-form [94669-40-6]
Cryst. (Et_2O/pet. ether or by subl.). Mp 97-99°. Bp_{11} 80° subl. . Hygroscopic.

Grob, C.A. *et al*, *Helv. Chim. Acta*, 1960, **43**, 1390 (*synth, uv*)
Tomer, K.B. *et al*, *Tetrahedron*, 1973, **29**, 3491 (*ms*)
Jefford, C.W. *et al*, *J. Org. Chem.*, 1977, **42**, 1654 (*synth*)
Hill, R.K. *et al*, *J. Org. Chem.*, 1985, **50**, 5528 (*synth, resoln, abs config*)
Demuth, M. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 4149 (*synth, resoln, cd*)
Lightner, D.A. *et al*, *J. Org. Chem.*, 1988, **53**, 1969 (*synth, ir, pmr, cmr, resoln, abs config*)

Bicyclo[3.2.1]oct-6-en-3-one B-80087

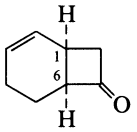
[3721-60-6]



$C_8H_{10}O$ M 122.166
Mp 100°. Bp_{11} 120-124° (Kugelrohr) .

Föhlisch, B. *et al*, *Chem. Ber.*, 1988, **121**, 1585 (*synth, pmr, cmr*)

Bicyclo[4.2.0]oct-2-en-7-one B-80088



(1*R*,6*S*)-*form*

$C_8H_{10}O$ M 122.166

(1R,6S)-form [52466-04-3]
(+)-cis-form
Volatile liq. Bp_{12} 65° (kugelrohr) . $[\alpha]_D^{25}$ +171.4° (0.47 in $CHCl_3$).

(1RS,6SR)-form [52466-03-2]
(±)-cis-form
Liq. Bp_{22} 85-90°.

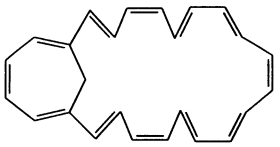
[34896-01-0]

Corey, E.J. *et al*, *Tetrahedron Lett.*, 1971, 4753 (*synth, ir*)
Kertesz, D.J. *et al*, *J. Org. Chem.*, 1988, **53**, 4962 (*synth, resoln, ms, pmr, cmr*)

Bicyclo[18.4.1]pentacosa-1,3,5,7,9,11,13,15,17,19,21,23-dodecaene, 9CI B-80089

1,6-Methano[24]annulene

[110977-31-6]



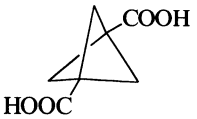
$C_{25}H_{24}$ M 324.465
Black needles (hexane). Mp 152-153°. Paratropic.

Yamamoto, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 395 (*synth, uv, ir, pmr*)

Bicyclo[1.1.1]pentane-1,3-dicarboxylic acid B-80090

Updated Entry replacing B-20094

[56842-95-6]



$C_7H_8O_4$ M 156.138
Solid. Subl. at 260-95° without melting.

Mono-Me ester: [83249-10-9].
$C_8H_{10}O_4$ M 170.165
Cryst. (heptane/$CHCl_3$). Mp 139.5-140°.

Di-Me ester: [115913-32-1].
$C_9H_{12}O_4$ M 184.191
Cryst. Mp 92°. Bp_{12} 125-130°.

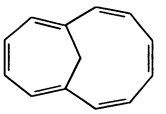
Dichloride: [115913-31-0].
$C_7H_6Cl_2O_2$ M 193.029
Mp 55-57°. Bp_{12} 120°.

Applequist, D.E. *et al*, *J. Org. Chem.*, 1982, **47**, 4985 (*synth*)
Kaszynski, P. *et al*, *J. Org. Chem.*, 1988, **53**, 4593 (*synth, derivs, ir, pmr, cmr, ms*)

Bicyclo[6.4.1]trideca-1,3,5,7,9,11-hexaene, 9CI B-80091

1,6-Methano[12]annulene

[52954-75-3]



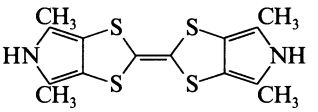
$C_{13}H_{12}$ M 168.238
Pale-yellow liq.

Yamamoto, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 395 (*synth, uv, pmr*)

2,2′-Bi(4,6-dimethyl-5*H*-1,3-dithiolo[4,5-*c*]pyrrolylidene) B-80092

*2-(4,6-Dimethyl-5*H*-1,3-dithiolo[4,5-*c*]pyrrol-2-ylidene)-5*H*-1,3-dithiolo[4,5-*c*]pyrrole, 9CI. Bis(2,5-dimethylpyrrolo[3,4-*d*]tetrathiafulvene)*

[117860-14-7]

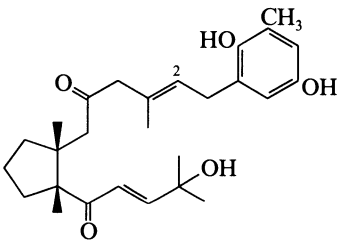


$C_{14}H_{14}N_2S_4$ M 338.542
Electron donor. Mp >300°.

Chen, W. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 7903 (*synth, pmr, ms, props*)

Bifurcarenone B-80093

Updated Entry replacing B-60105



$C_{27}H_{38}O_5$ M 442.594

(2E)-form
Constit. of *Cystoseira stricta*. Oil. $[\alpha]_D^{20}$ +5.5° (c, 8 in EtOH).

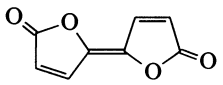
2′-Me ether:
$C_{28}H_{40}O_5$ M 456.621
Constit. of *C. stricta*. Oil. $[\alpha]_D^{20}$ +5.3° (c, 1.15 in EtOH).

(2Z)-form [75872-68-3]
Constit. of *Bifurcaria galapagensis*. Antibacterial. Oil. $[\alpha]_D$ −5.7° (c 0.34 in $CHCl_3$).

Sun, H.H. *et al*, *Tetrahedron Lett.*, 1980, 3123 (*isol, struct, spectra*)
Amico, V. *et al*, *Phytochemistry*, 1987, **26**, 1715 (*isol*)
Mori, K. *et al*, *Tetrahedron*, 1989, **45**, 1945 (*synth*)

2,2′-Bifurylidene-5,5′-dione B-80094

5-[5-Oxo-2(5H)-furanylidene]-2(5H)-furanone, 9CI



(*E*)-*form*

$C_8H_4O_4$ M 164.117

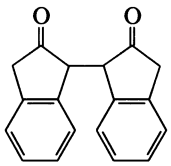
(***E***)-***form*** [15061-83-3]
V. pale yellow cryst. (AcOH). Mp 237° dec.

(***Z***)-***form*** [15061-82-2]
V. pale yellow cryst. Mp 248° dec.

Sauer, J.C. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 3677 (*synth, uv, ir, cryst struct*)

1,1′-Biindane-2,2′-dione B-80095

1,1′,3,3′-Tetrahydro-[1,1′-bi-2H-indene]-2,2′-dione, 9CI



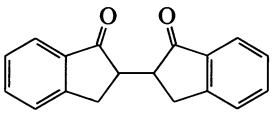
$C_{18}H_{14}O_2$ M 262.307
Mp 168° dec. Mixt. of *meso*- and (±)- stereoisomers.

[115679-36-2, 115679-45-3]

Baierweck, P. *et al*, *Chem. Ber.*, 1988, **121**, 2195 (*synth, pmr, cmr*)

2,2′-Biindane-1,1′-dione B-80096

2,2′,3,3′-Tetrahydro-[2,2′-bi-1H-indene]-1,1′-dione, 9CI



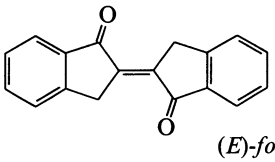
$C_{18}H_{14}O_2$ M 262.307
Mp 140°. Mixt. of *meso*- and (±)- isomers.

[115679-35-1, 115679-40-8]

Baierweck, P. *et al*, *Chem. Ber.*, 1988, **121**, 2195 (*synth, pmr, cmr*)

2,2′-Biindanylidene-1,1′-dione B-80097

2,3-Dihydro-2-(1,3-dihydro-1-oxo-2H-inden-2-ylidene)-1H-inden-1-one, 9CI



(*E*)-*form*

$C_{18}H_{12}O_2$ M 260.292

(***E***)-***form*** [115679-41-9]
Mp 225° dec.

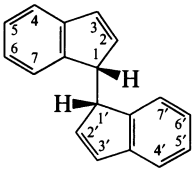
(***Z***)-***form*** [115679-38-4]
Cryst. (MeOH). Mp 200° dec.

Baierweck, P. *et al*, *Chem. Ber.*, 1988, **121**, 2195 (*synth, pmr, cmr*)

1,1′-Bi-1*H*-indene, 9CI B-80098

1,1′-Biindenyl

[2177-49-3]



(1*RS*,1′*RS*)-*form*

$C_{18}H_{14}$ M 230.309

(***1RS,1′RS***)-***form*** [81523-14-0]
(±)-*form*
Yellow needles (EtOH). Mp 99-100°.

(***1RS, 1′SR***)-***form*** [74339-76-7]
meso-*form*
Leaflets (Me_2CO). Mp 77.5°.

Lustenberger, P. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1979, **150**, 235 (*synth, cryst struct*)
Heimer, N.E. *et al*, *J. Org. Chem.*, 1982, **47**, 2593 (*synth, ir, pmr, cmr, abs config*)
Escher, A. *et al*, *Helv. Chim. Acta*, 1986, **69**, 1644 (*synth, uv, pmr, ms*)
Nicolet, P. *et al*, *Synthesis*, 1987, 202 (*synth, pmr*)

2,2′-Bi-1*H*-indene B-80099

2,2′-Biindenyl

$C_{18}H_{14}$ M 230.309
Leaflets (EtOH). Mp 252°.

Schroth, W. *et al*, *Z. Chem.*, 1963, **3**, 309 (*synth*)
Krauch, C.H. *et al*, *Chem. Ber.*, 1965, **98**, 2762 (*synth*)
Baierweck, P. *et al*, *Chem. Ber.*, 1988, **121**, 2195 (*synth, pmr, cmr*)

2,3′-Bi-1*H*-indene B-80100

2,3′-Biindenyl

[17252-90-3]

$C_{18}H_{14}$ M 230.309
Prisms (C_6H_6/pet.ether). Mp 220-224°.

Kemp, W. *et al*, *J. Chem. Soc. C*, 1967, 2544 (*synth, uv, ir*)

3,3′-Bi-1*H*-indene, 9CI B-80101

3,3′-Biindenyl

[7530-35-0]

$C_{18}H_{14}$ M 230.309
Cryst. (Ac_2O). Mp 131°.

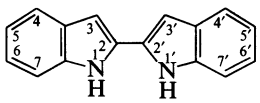
Ginsburg, D. *et al*, *J. Chem. Soc.*, 1961, 1498 (*synth, uv*)
Majerus, G. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 4147 (*synth, uv, ir*)
Höhn, J. *et al*, *Chem. Ber.*, 1983, **116**, 798 (*pmr, cmr*)
Nicolet, P. *et al*, *Synthesis*, 1987, 202 (*synth*)

2,2′-Bi-1*H*-indole, 9CI B-80102

Updated Entry replacing B-01208

2,2′-Biindolyl

[40899-99-8]

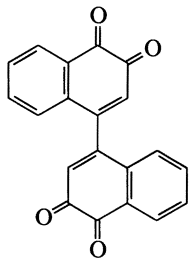


$C_{16}H_{12}N_2$ M 232.284
Cryst. (EtOAc). Mp 308-310°.

Faseeh, S.A. *et al*, *J. Chem. Soc.*, 1957, 4141 (*synth*)
Bergman, J. *et al*, *Tetrahedron*, 1979, **36**, 1439 (*ir, ms*)
Capuano, L. *et al*, *Chem. Ber.*, 1988, **121**, 2259 (*synth, pmr*)

4,4′-Bi(1,2-naphthaquinone) B-80103

[1,1′-Binaphthalene]-3,3′,4,4′-tetrone, 9CI
[64517-67-5]

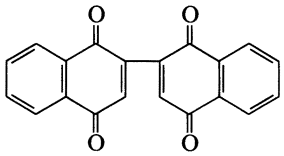


$C_{20}H_{10}O_4$ M 314.297
Yellow to orange-red cryst. Mp 289°.

Rosenhauer, E. *et al*, *Ber.*, 1937, **70**, 2281 (*synth*)
Paraskevas, S.M. *et al*, *Synthesis*, 1988, 897 (*synth, ir, pmr*)

2,2′-Bi(1,4-naphthoquinone) B-80104

[2,2′-Binaphthalene]-1,1′,4,4′-tetrone
[3408-13-7]

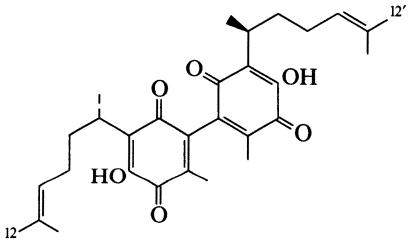


$C_{20}H_{10}O_4$ M 314.297
Yellow needles. Mp 273° dec.(darkens >270°).

Rosenhauer, E. *et al*, *Ber.*, 1937, **70**, 2281 (*synth*)
Paraskevas, S.M. *et al*, *Synthesis*, 1988, 897 (*synth, pmr, ir*)

Biperezone B-80105

[119318-13-7]



$C_{30}H_{38}O_6$ M 494.627
Constit. of *Coreocarpus arizonicus*.

12,12′-Bis(2-methylbutanoyloxy): [119285-24-4].
$C_{40}H_{54}O_{10}$ M 694.861
Constit. of *C. arizonicus*.

12,12′-Bis(3-methylbutanoyloxy): [119318-14-8].
$C_{40}H_{54}O_{10}$ M 694.861
Constit. of *C. arizonicus*.

Jolad, S.D. *et al*, *Phytochemistry*, 1988, **27**, 3545.

3,4′-Biphenyldiol B-80106

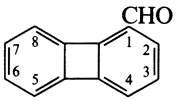
Updated Entry replacing B-01264
3,4′-Dihydroxybiphenyl
[18855-13-5]
$C_{12}H_{10}O_2$ M 186.210
Mp 197-198°.

Di-Me ether: 3,4′-Dimethoxybiphenyl
$C_{14}H_{14}O_2$ M 214.263
Mp 60-61°.

Ito, R. *et al*, *Bull. Chem. Soc. Jpn.*, 1963, **36**, 985 (*synth*)
Itoh, Y. *et al*, *Helv. Chim. Acta*, 1988, **71**, 1199 (*synth, deriv, ir, pmr*)

1-Biphenylenecarboxaldehyde B-80107

1-Formylbiphenylene
[1079-55-6]



$C_{13}H_8O$ M 180.206
Pale yellow cryst. Mp 44°.

2,4-Dinitrophenylhydrazone: [1103-51-1].
Orange cryst. Mp 287° dec.

Boulton, A.J. *et al*, *J. Chem. Soc. C*, 1968, 328 (*synth, ir, pmr*)

2-Biphenylenecarboxaldehyde B-80108

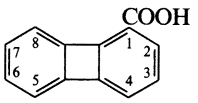
2-Formylbiphenylene
[65350-41-6]
$C_{13}H_8O$ M 180.206
Yellow cryst. (pet. ether). Mp 80-81°.

2,4-Dinitrophenylhydrazone: Deep red cryst. Mp 312-314° dec.

McOmie, J.F.W. *et al*, *J. Chem. Soc.*, 1962, 5298 (*synth, uv*)
Buckland, P.R. *et al*, *Tetrahedron*, 1977, **33**, 1797 (*synth*)
Kurosawa, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 3877 (*ir, pmr*)

1-Biphenylenecarboxylic acid B-80109

[17936-04-8]



$C_{13}H_8O_2$ M 196.205
Pale yellow plates (H_2O). Mp 224-225°.

Me ester: [1210-95-3].
$C_{14}H_{10}O_2$ M 210.232
Yellow needles. Mp 81°.

Nitrile: [35502-53-5]. *1-Cyanobiphenylene*
$C_{13}H_7N$ M 177.205
Yellow needles (hexane). Mp 59-59.5°.

Boulton, A.J. *et al*, *J. Chem. Soc. C*, 1968, 328 (*synth, deriv, uv*)
Barton, J.W. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 717 (*synth, deriv, ir*)

2-Biphenylenecarboxylic acid B-80110

[93103-69-6]
$C_{13}H_8O_2$ M 196.205
Yellow prisms (MeOH aq.). Mp 223-224°.

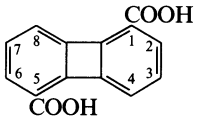
Me ester: [782-20-7].
$C_{14}H_{10}O_2$ M 210.232
Pale yellow plates (MeOH aq.). Mp 114-115°.

Chloride: [75292-39-6].
$C_{13}H_7ClO$ M 214.650
Yellow cryst. (C_6H_6). Mp 95.5-96.5°.

Nitrile: 2-Cyanobiphenylene
$C_{13}H_7N$ M 177.205
Yellow plates (pet. ether). Mp 99-100°.

Baker, W. *et al*, *J. Chem. Soc.*, 1954, 1476; 1958, 2666 (*synth, deriv, uv*)
Martin, R.H. *et al*, *Tetrahedron*, 1964, **20**, 2373 (*deriv, pmr*)
Droske, J.P. *et al*, *Macromolecules*, 1984, **17**, 10 (*synth, deriv*)

1,5-Biphenylenedicarboxylic acid B-80111



$C_{14}H_8O_4$ M 240.215
Polymer intermediate.

Di-Me ester: [20275-25-6].
$C_{16}H_{12}O_4$ M 268.268
Light yellow needles (Me_2CO). Mp 187-188°.

Dichloride: [81505-33-1].
$C_{14}H_6Cl_2O_2$ M 277.106
Yellow needles (C_6H_6/hexane). Mp 209-210°.

Newman, M.S. *et al*, *J. Org. Chem.*, 1971, 1398 (*synth, deriv, uv, ir, pmr*)
Sutter, A. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1982, **20**, 609 (*synth, deriv, ir, pmr*)

1,8-Biphenylenedicarboxylic acid B-80112

[119414-44-7]
$C_{14}H_8O_4$ M 240.215
Polymer intermediate. Yellow cryst.

Di-Me ester: [20275-26-7].
$C_{16}H_{12}O_4$ M 268.268
Yellow needles (EtOH). Mp 147-148°.

Dichloride: [81505-34-2].
$C_{14}H_6Cl_2O_2$ M 277.106
Yellow plates (hexane). Mp 139-140°.

Newman, M.S. *et al*, *J. Org. Chem.*, 1971, **36**, 1398 (*synth, deriv, uv, ir, pmr*)
Sutter, A. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1982, **20**, 609 (*synth, deriv, ir, pmr*)
Wilcox, C.F. *et al*, *J. Org. Chem.*, 1989, **54**, 2190 (*synth*)

2,3-Biphenylenedicarboxylic acid B-80113

$C_{14}H_8O_4$ M 240.215

Di-Me ester: [84509-69-3].
$C_{16}H_{12}O_4$ M 268.268
Yellow cryst. (cyclohexane). Mp 80-81°.

Berris, B.C. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 5670 (*synth, uv, ir, pmr, ms*)

2,6-Biphenylenedicarboxylic acid B-80114

[65330-85-0]
$C_{14}H_8O_4$ M 240.215
Polymer intermediate. Mp 350° dec.

Di-Me ester: [67278-30-2].
$C_{16}H_{12}O_4$ M 268.268
Cryst. (C_6H_6). Mp 223-225°.

Dichloride: [65330-84-9].
$C_{14}H_6Cl_2O_2$ M 277.106
Cryst. (C_6H_6). Mp 242-244°.

Swedo, R.J. *et al*, *J. Polym. Sci., Polym. Lett. Ed.*, 1977, **15**, 683 (*synth*)
Recca, A. *et al*, *Macromolecules*, 1978, **11**, 479 (*synth, ir*)
Sutter, A. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1982, **20**, 609 (*synth*)
Sato, M. *et al*, *Tetrahedron Lett.*, 1984, **25**, 3603 (*synth*)

2,7-Biphenylenedicarboxylic acid B-80115

[69417-80-7]
$C_{14}H_8O_4$ M 240.215
Polymer intermediate. Yellow solid. Mp 354-360°.

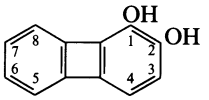
Di-Me ester: [69417-79-4].
$C_{16}H_{12}O_4$ M 268.268
Yellow cryst. (Me_2CO). Mp 190-193°.

Dichloride: [69417-81-8].
$C_{14}H_6Cl_2O_2$ M 277.106
Yellow needles (C_6H_6/hexane). Mp 197-198°.

Hanson, M.P. *et al*, *J. Polym. Sci., Polym. Lett. Ed.*, 1978, **16**, 653 (*synth, uv*)
Sutter, A. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1982, **20**, 609 (*synth, ir, pmr*)

1,2-Biphenylenediol, 9CI B-80116

1,2-Dihydroxybiphenylene



$C_{12}H_8O_2$ M 184.194

O^2-*Me:* [63723-84-2]. *2-Methoxy-1-biphenylenol. 1-Hydroxy-2-methoxybiphenylene*
$C_{13}H_{10}O_2$ M 198.221
Yellow needles. Mp 94-95°.

Di-Me ether: [63723-85-3]. *1,2-Dimethoxybiphenylene*
$C_{14}H_{12}O_2$ M 212.248
Yellowish leaflets (EtOH). Mp 132.5-133.5°.

Sato, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 2334 (*synth, ir, ms, pmr*)

1,5-Biphenylenediol, 9CI B-80117

1,5-Dihydroxybiphenylene
[98991-02-7]
$C_{12}H_8O_2$ M 184.194
Cryst. ($CHCl_3$). Mp 266-268°.

Di-Me ether: [98991-11-8]. *1,5-Dimethoxybiphenylene*
$C_{14}H_{12}O_2$ M 212.248
Pale yellow cryst. (CH_2Cl_2/hexane). Mp 153-155°.

[98991-11-8]
Hine, J. *et al*, *J. Org. Chem.*, 1985, **50**, 5092 (*synth, pmr*)

1,8-Biphenylenediol B-80118

1,8-Dihydroxybiphenylene
[18798-64-6]
$C_{12}H_8O_2$ M 184.194
Straw-coloured prisms (C_6H_6). Mp 223-224°.

Di-Ac: [18798-65-7].
$C_{16}H_{12}O_4$ M 268.268
Needles (hexane). Mp 136-137°.

Blatchly, J.M. *et al*, *J. Chem. Soc. C*, 1968, 1545 (*synth, uv, pmr*)
Hine, J. *et al*, *J. Org. Chem.*, 1986, **51**, 577; 1987, **52**, 2083 (*props, uv*)

2,3-Biphenylenediol B-80119

2,3-Dihydroxybiphenylene
$C_{12}H_8O_2$ M 184.194

Di-Me ether: 2,3-Dimethoxybiphenylene
$C_{14}H_{12}O_2$ M 212.248
Yellow needles by subl. Mp 87-88°. Bp_{12} 85° subl.

Blatchly, J.M. *et al*, *J. Chem. Soc.*, 1962, 5085, 5090 (*synth, uv*)

2,6-Biphenylenediol B-80120

2,6-Dihydroxybiphenylene

$C_{12}H_8O_2$ M 184.194

Di-Ac: [13625-15-5].
$C_{16}H_{12}O_4$ M 268.268
Faint yellow plates (AcOH), cryst. (Me_2CO). Mp 220° dec.

Di-Me ether: [13625-14-4]. *2,6-Dimethoxybiphenylene*
$C_{14}H_{12}O_2$ M 212.248
Lemon yellow plates or needles (MeOH). Mp 132-133°.

Blatchly, J.M. *et al*, *J. Chem. Soc. C*, 1967, 272 (*synth*, *uv*, *ir*)

2,7-Biphenylenediol, 9CI B-80121

2,7-Dihydroxybiphenylene

$C_{12}H_8O_2$ M 184.194

Di-Ac: [13625-17-7].
$C_{16}H_{12}O_4$ M 268.268
Needles (hexane), cryst. (EtOH aq.). Mp 141-143°.

Me ether, Ac: [18798-63-5].
$C_{15}H_{12}O_3$ M 240.258
Yellow needles (EtOH aq.). Mp 95.5-96°.

Di-Me ether: [18798-68-0]. *2,7-Dimethoxybiphenylene, 9CI*
$C_{14}H_{12}O_2$ M 212.248
Bright yellow plates (Et_2O, EtOH, or pentane). Mp 107.5-109°. Bp_{12} 130° subl.

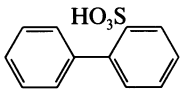
Di-Me ether, picrate: Red-black cryst. (EtOH). Mp 125°.

Lothrop, W.C., *J. Am. Chem. Soc.*, 1942, **64**, 1698 (*synth*, *deriv*)
Baker, W. *et al*, *J. Chem. Soc.*, 1958, 2688; 1961, 3986 (*synth*, *uv*, *deriv*)
Farnum, D.G. *et al*, *J. Org. Chem.*, 1961, **26**, 3204 (*uv*, *props*, *deriv*)
Blatchly, J.M. *et al*, *J. Chem. Soc. C*, 1967, 272; 1968, 1545 (*synth*, *uv*, *pmr*, *ir*, *derivs*)

[1,1′-Biphenyl]-2-sulfonic acid B-80122

2-Phenylbenzenesulfonic acid

[19813-86-6]



$C_{12}H_{10}O_3S$ M 234.275
Cryst. (tetrachloroethane). Mp 94°.

Me ester:
$C_{13}H_{12}O_3S$ M 248.302
Cryst (pet. ether). Mp 83.5-85°.

Chloride:
$C_{12}H_9ClO_2S$ M 252.721
Cryst. (hexane/$CHCl_3$). Mp 103°.

Dannley, R.L. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2997 (*ester*)
Zaraiskii, A.P. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1973, **9**, 1017 (*synth*)

[1,1′-Biphenyl]-3-sulfonic acid, 9CI B-80123

3-Phenylbenzenesulfonic acid

[41949-30-8]

$C_{12}H_{10}O_3S$ M 234.275
Cryst. Mp 38-40°.

Me ester:
$C_{13}H_{12}O_3S$ M 248.302
$Bp_{0.3}$ 150-160°.

Chloride:
$C_{12}H_9ClO_2S$ M 252.721
Cryst. Mp 44° (37-40°).

Amide:
$C_{12}H_{11}NO_2S$ M 233.290
Cryst. Mp 131° (121°).

Finzi, C. *et al*, *Ann. Chim.* (*Rome*), 1950, **40**, 334 (*synth*)
Dannley, R.L. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2997 (*ester*)
Zaraiskii, A.P. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1973, **9**, 1017 (*synth*)

[1,1′-Biphenyl]-4-sulfonic acid, 9CI B-80124

4-Phenylbenzenesulfonic acid

[2113-68-0]

$C_{12}H_{10}O_3S$ M 234.275
Cryst. Mp 138° (117-119°).

Me ester:
$C_{13}H_{12}O_3S$ M 248.302
Cryst. (pet.ether). Mp 76-77°.

Chloride: [1623-93-4].
$C_{12}H_9ClO_2S$ M 252.721
Mp 115°, Mp 142-143°.

Amide:
$C_{12}H_{11}NO_2S$ M 233.290
Cryst. Mp 228°.

Gebauer-Fülnegg, E. *et al*, *Monatsh. Chem.*, 1928, **49**, 46 (*chloride*)
Pollak, J. *et al*, *Monatsh. Chem.*, 1930, **35**, 358 (*synth*)
Dannley, R.L. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2997 (*ester*)
Schultz, R.G., *J. Org. Chem.*, 1961, **26**, 5195 (*synth*)
Roemmele, R.C. *et al*, *J. Org. Chem.*, 1988, **53**, 2367 (*synth*, *pmr*, *ir*)

2,2′,3,4-Biphenyltetrol B-80125

2,2′,3,4-Tetrahydroxybiphenyl

$C_{12}H_{10}O_4$ M 218.209

Tetra-Me ether: [119101-10-9]. *2,2′,3,4-Tetramethoxybiphenyl*
$C_{16}H_{18}O_4$ M 274.316
Cryst. (diisopropyl ether). Mp 105°.

Itoh, Y. *et al*, *Helv. Chim. Acta*, 1988, **7**, 1199 (*synth*, *pmr*)

2,3,3′,4-Biphenyltetrol B-80126

Updated Entry replacing B-01303

2,3,3′,4-Tetrahydroxybiphenyl

$C_{12}H_{10}O_4$ M 218.209

Tetra-Me ether: 2,3,3′,4-Tetramethoxybiphenyl
$C_{16}H_{18}O_4$ M 274.316
Cryst. (MeOH). Mp 96-100°. Also descr. as oil.

Goto, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1941, **16**, 170 (*synth*)
Itoh, Y. *et al*, *Helv. Chim. Acta*, 1988, **71**, 1199 (*synth*, *deriv*, *ir*, *pmr*)

2,3,4,4′-Biphenyltetrol B-80127

2,3,4,4′-Tetrahydroxybiphenyl

$C_{12}H_{10}O_4$ M 218.209

Tetra-Me ether: [6271-59-6]. *2,3,4,4′-Tetramethoxybiphenyl*
$C_{16}H_{18}O_4$ M 274.316
Cryst. (diisopropyl ether). Mp 75°.

Itoh, Y. *et al*, *Helv. Chim. Acta*, 1988, **71**, 1199 (*synth*, *pmr*)

2,3′,4′,5′-Biphenyltetrol B-80128

Updated Entry replacing B-20101

2,3′,4′,5′-Tetrahydroxybiphenyl

$C_{12}H_{10}O_4$ M 218.209
Mp 150-151.5°.

2,3′,5′-Tri-Me ether: 2,6-Dimethoxy-4-(2-methoxyphenyl)phenol. 4-Hydroxy-2′,3,5-

$C_{15}H_{16}O_4$ M 260.289
Constit. of the heartwood of *Sorbus aucuparia* and *S. decora*. Mp 120-122°.

Tetra-Me ether: 2′,3,4,5-Tetramethoxybiphenyl
$C_{16}H_{18}O_4$ M 274.316
Cryst. (MeOH aq.). Mp 71.5-72°.

Erdtman, H. *et al*, *Acta Chem. Scand.*, 1963, **17**, 1151 (*synth, uv*)
Nilsson, M. *et al*, *Acta Chem. Scand.*, 1963, **17**, 1157 (*Methoxyaucuparin*)

3,4,5-Biphenyltriol, 8CI B-80129

Updated Entry replacing B-01332
5-Phenylpyrogallol. 3,4,5-Trihydroxybiphenyl
$C_{12}H_{10}O_3$ M 202.209
Cryst. (MeOH aq.). Mp 196-198°.

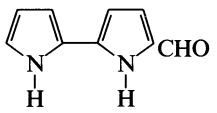
3,5-Di-Me ether: 3,5-Dimethoxy-4-biphenylol. 4-Hydroxy-3,5-dimethoxybiphenyl. ***Aucuparin***
$C_{14}H_{14}O_3$ M 230.263
Isol. from trunkwood of *Sorbus aucuparia*. Cryst. Mp 101-101.5°.

Tri-Me ether: [50816-75-6]. *3,4,5-Trimethoxybiphenyl*
$C_{15}H_{16}O_3$ M 244.290
Cryst. (MeOH). Mp 84-89°.

Narasimhachari, N. *et al*, *Can. J. Chem.*, 1962, **40**, 1118 (*isol, deriv*)
Erdtman, H. *et al*, *Acta Chem. Scand.*, 1963, **17**, 1151 (*uv, pmr*)
Nilsson, M. *et al*, *Acta Chem. Scand.*, 1963, **17**, 1157 (*synth*)

2,2′-Bi-1*H*-pyrrole-5-carboxaldehyde B-80130

5-Formyl-2,2′-bipyrrole
[22187-87-7]

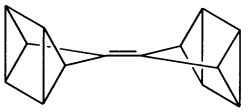


$C_9H_8N_2O$ M 160.175
Cryst. (EtOH aq.). Mp 234-240° dec.

Hearn, W.R. *et al*, *J. Org. Chem.*, 1970, **35**, 142 (*synth, uv, pmr, ms*)
Boger, D.L. *et al*, *J. Org. Chem.*, 1988, **53**, 1405 (*synth, ir, pmr, ms*)

Biquadricyclenylidene B-80131

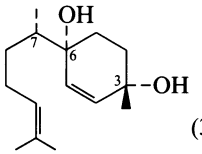
3-Tetracyclo[3.2.0.0^{2,7}.0^{4,6}]hept-3-ylidenetetracyclo[3.2.0.0^{2,7}0^{4,6}]heptane, 9CI
[53312-09-7]



$C_{14}H_{12}$ M 180.249
Prisms. Mp 173° subl.

Sauter, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1973, **12**, 991 (*synth, pmr*)
Knothe, L. *et al*, *Justus Liebigs Ann. Chem.*, 1977, 709 (*cmr*)
Prinzbach, H. *et al*, *Tetrahedron Lett.*, 1981, **22**, 2541 (*struct*)
Trah, S. *et al*, *Tetrahedron Lett.*, 1987, **28**, 4399, 4403 (*struct*)

1,10-Bisabolene-3,6-diol B-80132



(3*R*,6*R*,7*S*)-*form*

$C_{15}H_{26}O_2$ M 238.369
Incorrect numbering system used in reference.

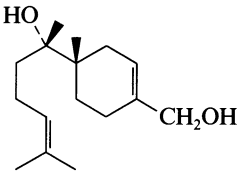
(3R,6R,7S)-form [119285-25-5]
Constit. of *Coreocarpus arizonicus*. Oil.

(3S,4S,7S)-form [119364-23-7]
Constit. of *C. arizonicus*. Oil.

Jolad, S.D. *et al*, *Phytochemistry*, 1988, **27**, 3545.

3,10-Bisaboladiene-7,14-diol B-80133

[116537-80-5]

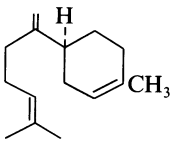


$C_{15}H_{26}O_2$ M 238.369
Constit. of *Vanillosmopsis arborea*. Oil.

Matos, M.E.O. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 780.

β-Bisabolene B-80134

Updated Entry replacing B-40083
1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)cyclohexene, 9CI



(*S*)-*form*
Absolute configuration

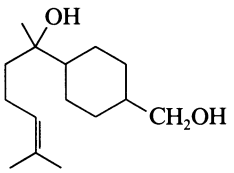
$C_{15}H_{24}$ M 204.355

(R)-form
Isol. from *Chamaecyparis nootkatensis* and *Pinus sibirica*. $[\alpha]_D$ +75°. n_D^{20} 1.4879.

(S)-form [495-61-4]
Constit. of the essential oils of bergamot, lemon and wild carrot. Oil. $Bp_{10.5}$ 129-130°. $[\alpha]_D^{20}$ −84.4°.

Pentegova, V.A. *et al*, *Collect. Czech. Chem. Commun.*, 1961, **26**, 1362 (*isol*)
Manjarrez, A. *et al*, *J. Org. Chem.*, 1966, **31**, 348 (*synth*)
Andersen, N.H. *et al*, *Phytochemistry*, 1970, **9**, 1325 (*isol*)
Vig, O.P. *et al*, *J. Indian Chem. Soc.*, 1971, **48**, 993 (*synth*)
Crawford, R.J. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 4298 (*synth*)
Sakane, S. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 6154 (*synth*)
Sakurai, H. *et al*, *Tetrahedron*, 1983, **39**, 883 (*synth*)
Nabeta, K. *et al*, *Agric. Biol. Chem.*, 1986, **50**, 2915 (*biosynth*)

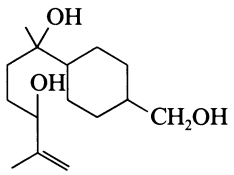
10-Bisabolene-7,15-diol B-80135



$C_{15}H_{28}O_2$ M 240.385
Constit. of *Baccharis latifolia*. Oil.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

11-Bisabolene-7,10,15-triol B-80136

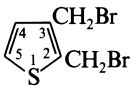


$C_{15}H_{28}O_3$ M 256.384
Constit. of *Baccharis latifolia*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

2,3-Bisbromomethyl)thiopene B-80137

[13250-86-7]



$C_6H_6Br_2S$ M 269.987
Cryst. (hexane). Mp 49-50°.

MacDowell, D.W.H. *et al*, *J. Org. Chem.*, 1966, **31**, 3592 (*synth, ir, uv, pmr*)
Chadwick, D.J. *et al*, *Tetrahedron Lett.*, 1987, **28**, 6085 (*synth*)

2,5-Bis(bromomethyl)thiophene B-80138

[59311-25-0]

$C_6H_6Br_2S$ M 269.987
Cryst. (pet. ether). Mp 78°.

Clarke, J.A. *et al*, *Tetrahedron Lett.*, 1975, 4183 (*synth*)
Bilger, C. *et al*, *Synthesis*, 1988, 902 (*synth, ms, ir, pmr*)

3,4-Bis(bromomethyl)thiophene B-80139

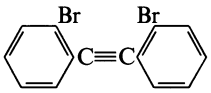
[38447-31-3]

$C_6H_6Br_2S$ M 269.987
Cryst. (cyclohexane/pet. ether). Mp 83°.

Von Reinhard, H., *J. Prakt. Chem.*, 1972, **314**, 334 (*synth, nmr*)

Bis(2-bromophenyl)ethyne B-80140

2,2'-Dibromotolan. 2,2'-Dibromodiphenylacetylene



$C_{14}H_8Br_2$ M 336.025
Cryst. (EtOH). Mp 81.0-81.5°.

Letsinger, R.L., *J. Am. Chem. Soc.*, 1959, **81**, 3013 (*synth, ir*)

Bis(4-bromophenyl)ethyne B-80141

4,4'-Dibromotolan. 4,4'-Dibromodiphenylacetylene

$C_{14}H_8Br_2$ M 336.025
Cryst. ($CHCl_3$). Mp 184.5-185°.

Misumi, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1962, **35**, 135 (*synth*)

Bis(chlorocarbonyl) disulfide B-80142

Dithiobis(carbonylchloride). Thioperoxydicarbonic dichloride, 9CI

[51615-88-4]

ClCO-S-S-COCl

$C_2Cl_2O_2S_2$ M 191.058
Liq. Bp_{20} 84°. Stable to storage if kept dry.

Kobayashi, N. *et al*, *Chem. Lett.*, 1973, 1315 (*synth*)
Haas, A. *et al*, *J. Fluorine Chem.*, 1973, **3**, 383 (*synth, ir, ms*)
Barany, G. *et al*, *J. Org. Chem.*, 1983, **48**, 4750 (*synth*)

2,4-Bis(chloromethyl)pyridine B-80143

[101822-23-5]

$C_7H_7Cl_2N$ M 176.044
Red oil.

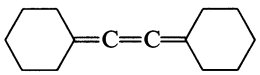
[120492-00-4]

Kawashima, T. *et al*, *Chem. Lett.*, 1988, 1707.
Przybilla, K.J. *et al*, *Chem. Ber.*, 1989, **122**, 347 (*synth, pmr*)

1,2-Bis(cyclohexylidene)ethene B-80144

1,1'-(1,2-Ethenediylidene)biscyclohexane, 9CI. 1,4-Bis(pentamethylene)-1,2,3-butatriene

[36204-35-0]



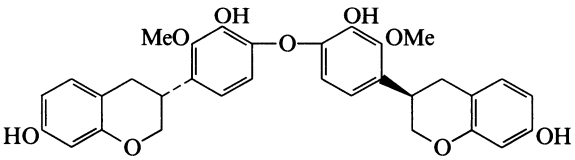
$C_{14}H_{20}$ M 188.312
Cryst. by subl. Mp 81.5-82.0°. Unstable in air, can be stored in CCl_4 or hexane soln. under Ar.

Iyoda, M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 8494 (*synth, pmr, cmr, uv, ir*)

Biscyclolobin B-80145

3,3'-[Oxybis(3-hydroxy-2-methoxy-4,1-phenylene)]-bis[3,4-dihydro-2H-1-benzopyran-7-ol], 9CI

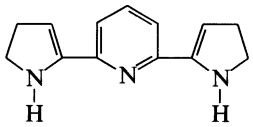
[58219-01-5]



$C_{32}H_{30}O_9$ M 558.584
Isol. from heartwood of *Cyclobium clausseni*. Mp 220-223°.

Gottlieb, O.R. *et al*, *Phytochemistry*, 1975, **14**, 2495 (*isol, uv, ms, ord, struct*)

2,6-Bis(3,4-Dihydro-2*H*-pyrrol-5-yl) pyridine B-80146

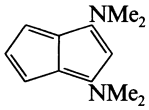


$C_{13}H_{15}N_3$ M 213.282
Cryst. (H_2O). Mp 132°.

Bernauer, K. *et al*, *Helv. Chim. Acta*, 1989, **72**, 477 (*synth*, *pmr*)

1,3-Bis(dimethylamino)pentalene B-80147

N,N,N′,N′-*Tetramethyl-1,3-pentalenediamine*, *8CI*
[14749-76-9]

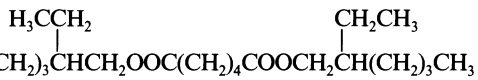


$C_{12}H_{16}N_2$ M 188.272
Simple stabilised pentalene. Dark-blue cryst. Mp 163° dec. Stable in air for several hr. at r.t.

Hafner, K. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1967, **6**, 451 (*synth*, *uv*, *pmr*)
Eckert-Maksić, M. *et al*, *Chem. Ber.*, 1988, **121**, 1219 (*pe*)

Bis(2-ethylhexyl)adipate B-80148

Diethylhexyl adipate. DEHA
[103-23-1]



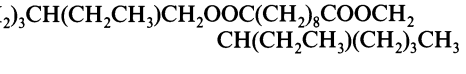
$C_{22}H_{42}O_4$ M 370.571
Plasticizer; used as component in lube oils. Liq. d_4^{20} 0.927. Bp_2 181-5°. Pour point −70°, glass point −112°. n_D^{20} 1.447.

▷ May be carcinogenic, mutagenic.

Klamann, D. *et al*, *Brennst.-Chem.*, 1964, **45**, 33; *CA*, **60**, 13137e (*synth*)
Cornell, R.R. *et al*, *Arch. Mass Spectral Data*, 1971, **2**, 710 (*ms*)
Takahashi, T. *et al*, *Toxicology*, 1981, **22**, 223; *CA*, **96**, 80969t (*tox*)
Ovchinnikov, E.Yu. *et al*, *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1985, **59**, 1693 (*props*)
Castle, L. *et al*, *J. Assoc. Off. Anal. Chem.*, 1988, **71**, 394 (*glc*, *ms*)

Bis(2-ethylhexyl) decanedioate B-80149

Bis(2-ethylhexyl) sebacate. Di(2-ethylhexyl) sebacate
[122-62-3]

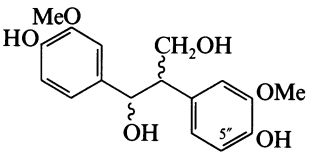


$C_{26}H_{50}O_4$ M 426.679
Used in inks, lubricating oils, hydraulic fluids, plasticizers, coatings. Glc stationary phase. Liq. Sol. EtOH, C_6H_6, Me_2CO. d_4^{20} 0.914. Mp −48°. Bp_5 256°. n_D^{25} 1.4496. The coml. prod. will be a mixt. of diastereoisomers expected to have v. similar props.

Durr, A.M. *et al*, *ACS Div. Petrol. Chem. Preprints*, 1963, **8**, 49 (*synth*, *props*)
Reith, H. *et al*, *CA*, 1963, **59**, 11159b (*props*)
Wood, G.M. *et al*, *J. Vac. Sci. Technol.*, 1969, **6**, 871; *CA*, **71**, 126859w (*ms*)
Fr. Pat., 2 151 525, (1973); *CA*, **79**, 52813t (*synth*, *purifn*)
Reglero, G. *et al*, *Chromatographia*, 1986, **22**, 358 (*glc*)

1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol, 8CI B-80150

1,2-Diguaiacyl-1,3-propanediol
[4206-59-1]



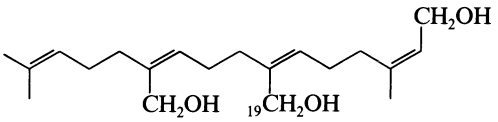
$C_{17}H_{20}O_6$ M 320.341
Obt. by mild hydrol. of wood of *Fagus sylvatica* and *Picea excelsa*. Prisms (EtOH aq.). Mp 143.5°.

5″-Methoxy: ***1-(4-Hydroxy-3-methoxyphenyl)-2-(4-hydroxy-3,5-dimethoxyphenyl)-1,3-propanediol***
$C_{18}H_{22}O_7$ M 350.368
Obt. by mild hydrol. of lignin of *F. sylvatica*. Needles (MeOH aq.). Mp 192-193°.

Nimz, H., *Chem. Ber.*, 1966, **99**, 469.

7,11-Bis(hydroxymethyl)-3,15-dimethyl-2,6,10,14-hexadecatetraen-1-ol B-80151

18,19-Dihydroxygeranylnerol

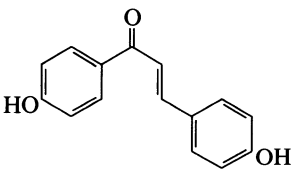


$C_{20}H_{34}O_3$ M 322.487
19-Ac: 19-Acetoxy-18-hydroxygeranylnerol
$C_{22}H_{36}O_4$ M 364.524
Constit. of *Ageratina ligustrina*. Oil.

Tamayo-Catillo, G. *et al*, *Phytochemistry*, 1988, **27**, 2893.

1,3-Bis(4-hydroxyphenyl)-2-propen-1-one B-80152

4,4′-Dihydroxychalcone
[108997-30-4]

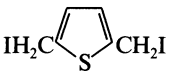


$C_{15}H_{12}O_3$ M 240.258
Constit. of *Chamaecyparis obtusa*. Yellow needles (MeOH aq.). Mp 207-208°.

Klinke, P. *et al*, *Chem. Ber.*, 1961, **94**, 26 (*synth*)
Ohashi, H. *et al*, *Phytochemistry*, 1988, **27**, 3993 (*isol*)

2,5-Bis(iodomethyl)thiophene B-80153

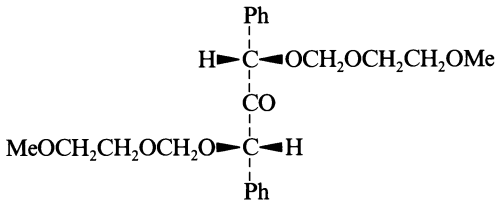
[120651-39-0]



$C_6H_6I_2S$ M 363.988
Solid. Unstable, must be used immediately.

Bilger, C. *et al*, *Synthesis*, 1988, 902 (*synth*)

1,3-Bis[(2-methoxyethoxy)methoxy]-1,3-diphenyl-2-propanone B-80154



$C_{23}H_{30}O_7$ M 418.486
Readily available C_2-symmetric ketone for asymmetric synthesis.

(S,S)-form [119945-33-4]
$[\alpha]_D^{25}$ +212.4° (c, 0.58 in 95% EtOH aq.). *meso*-form also obt.

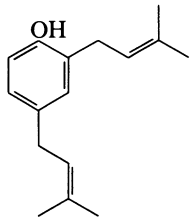
[119909-46-5]

Braun, M. *et al*, *Chem. Ber.*, 1989, **122**, 1215 (*synth, ir, pmr*)

2,4-Bis(3-methyl-2-butenyl)phenol B-80155

2,4-Diprenylphenol

[55824-31-2]



$C_{16}H_{22}O$ M 230.349
Constit. of *Perithalia caudata*. Oil.

Kyogoku, K. *et al*, *Agric. Biol. Chem.*, 1975, **39**, 133 (*synth*)
Yamada, S. *et al*, *Synth. Commun.*, 1975, **5**, 181 (*synth*)
Blackmann, A.J. *et al*, *Phytochemistry*, 1988, **27**, 3686 (*isol*)

3,3-Bis(methylthio)propenal B-80156

[78263-38-4]

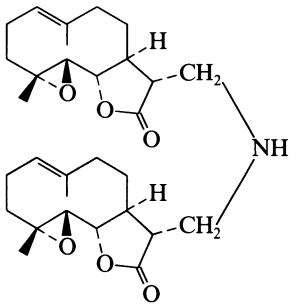
$$(MeS)_2C{=}CHCHO$$

$C_5H_8OS_2$ M 148.250

Dieter, R.K. *et al*, *J. Org. Chem.*, 1988, **53**, 2031 (*synth, ir, pmr, cmr*)

Bisparthenolidine B-80157

[112078-76-9]



$C_{30}H_{43}NO_6$ M 513.673

Constit. of *Paramichelia baillonii* and *Michelia rajaniana* (Magnoliaceae). Cryst. ($CHCl_3$). Mp 100-103°. $[\alpha]_D^{20}$ −112° ($CHCl_3$).

Ruangrungsi, N. *et al*, *J. Nat. Prod.* (*Lloydia*), 1987, **50**, 891; 1988, **51**, 1230 (*isol, pmr, cmr*)

Bis(pentafluorophenyl)methane B-80158

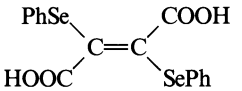
[5736-46-9]

$$(C_6F_5)_2CH_2$$

$C_{13}H_2F_{10}$ M 348.143
Cryst. by subl. Mp 63-64°.

Beckert, W.F. *et al*, *J. Org. Chem.*, 1967, **32**, 582 (*synth, ir, F nmr*)
Filler, R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 287 (*props*)
Bordwell, F.G. *et al*, *J. Org. Chem.*, 1988, **53**, 780 (*synth, pmr*)

2,3-Bis(phenylseleno)-2-butenedioic acid B-80159



(E)-form

$C_{16}H_{12}O_4Se_2$ M 426.188

(E)-form [114221-67-9]
Pale yellow cryst. (Me_2CO/hexane). Mp 240-246°.

Di-Me ester: [114221-61-3].
$C_{18}H_{16}O_4Se_2$ M 454.242
Pale yellow solid ($CHCl_3$/hexane). Mp 109.5-110°.

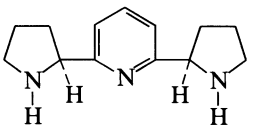
(Z)-form [114221-68-0]
Bright yellow solid. Mp 169-172°.

Di-Me ester: [114221-62-4].
Bright yellow solid ($CHCl_3$/hexane). Mp 117-118.5°.

Anhydride: [114221-69-1].
$C_{16}H_{10}O_3Se_2$ M 408.173
Bright yellow gum.

Back, T.G. *et al*, *J. Org. Chem.*, 1988, **53**, 2533 (*synth, ir, pmr, ms*)

2,6-Bis(2-pyrrolidinyl)pyridine B-80160



(R,R*)-form*

$C_{13}H_{19}N_3$ M 217.313
Tridentate ligand. $Bp_{0.005}$ 96°. Bp refers to a mixt. of (±)- and *meso*-isomers, not separately characterised. The (±)-form was resolved.

(R*,R*)-form
(+)-*form*
$[\alpha]_D$ +126° (c, 0.1 in H_2O).

(S*,S*)-form
(−)-*form*
$[\alpha]_D$ −113°.

Bernauer, K. *et al*, *Helv. Chim. Acta*, 1989, **72**, 477 (*synth, uv, pmr, resoln*)

[Bis(trifluoroacetoxy)iodo]pentafluorobenzene B-80161

*(Pentafluorophenyl)bis(trifluoroacetato-*O*)-iodine, 9CI*

[14353-88-9]

$$C_6F_5I(OOCCF_3)_2$$

$C_{10}F_{11}IO_4$ M 519.994
Reagent for mild oxidative cleavage of alkynes and carbonyl compds. Cryst. by subl. Mp 119-120°.

Schmeisser, M. *et al*, *Chem. Ber.*, 1967, **100**, 1633 (*synth*)
Moriarty, R.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 202 (*use*)
Moriarty, R.M. *et al*, *J. Org. Chem.*, 1988, **53**, 6124 (*use*)

Bis(trifluoromethyl)sulfene B-80162

$(F_3C)_2C{=}SO_2$

$C_3F_6O_2S$ M 214.088
Quinuclidine adduct: [118724-94-0].
Cryst. Mp 181° dec.

Hartwig, U. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 221 (*synth, cryst struct*)

Bis[(trifluoromethyl)thio]acetylene, 8CI B-80163

[2069-87-6]

$F_3CSC{\equiv}CSCF_3$

$C_4F_6S_2$ M 226.166
Liq. Bp 83°. n_D^{25} 1.3924. Slowly darkens on standing.

Harris, J.F., *J. Org. Chem.*, 1967, **32**, 2063 (*synth, ir*)
Haas, A. *et al*, *Chem. Ber.*, 1988, **121**, 1833 (*synth, cmr*)

1,2-Bis[(trifluoromethyl)thio]ethene, 9CI B-80164

$F_3CSCH{=}CHSCF_3$

$C_4H_2F_6S_2$ M 228.182
Liq. Bp 92-98°. Geom. isomers separable by glc.

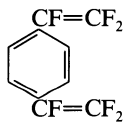
[13003-45-7, 13003-46-8]

Harris, J.F., *J. Org. Chem.*, 1967, **32**, 2063 (*synth, ir, uv*)

1,4-Bis(trifluorovinyl)benzene B-80165

1,4-Bis(trifluoroethenyl)benzene

[113268-53-4]



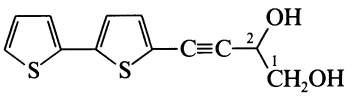
$C_{10}H_4F_6$ M 238.132
Liq. Pure product readily dimerises.

Heinze, P.L. *et al*, *J. Org. Chem.*, 1988, **53**, 2714 (*synth, F nmr, pmr, ir, ms*)

4-[2,2′-Bithiophen]-5-yl-3-butyne-1,2-diol, 9CI B-80166

5-(3,4-Dihydroxy-1-butynyl)-2,2′-bithienyl

[1211-45-6]



$C_{12}H_{10}O_2S_2$ M 250.342
Isol. from roots of *Echinops sphaerocephalus*. Cryst. (CCl_4/Et_2O). Mp 102°. $[\alpha]_{546}^{25}$ +12° (c, 2.55 in Et_2O).

O^1-Ac: 5-(3-Hydroxy-4-acetoxy-1-butynyl)-2,2′-bithienyl
$C_{14}H_{12}O_3S_2$ M 292.379
Isol. from *E. sphaerocephalus*. Oil. λ_{max} 325,332 nm.

O^2-Ac: [95910-62-6]. *5-(4-Hydroxy-3-acetoxy-1-butynyl)-2,2′-bithienyl.* ***α-Tertiophene***
$C_{14}H_{12}O_3S_2$ M 292.379
Isol. from *E. sphaerocephalus*.

Di-Ac: [1233-95-0]. *5-(3,4-Diacetoxy-1-butynyl)-2,2′-bithienyl*
$C_{16}H_{14}O_4S_2$ M 334.416
Isol. from *E. sphaerocephalus* and *Tagetes patula*. Oil. $[\alpha]_{546}^{25}$ +183° (c, 0.89 in Et_2O).

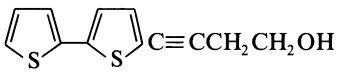
Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 155, 876 (*isol, uv, ir, pmr, ord, struct, biosynth*)
Pensl, R. *et al*, *Z. Naturforsch., C*, 1985, **40**, 3 (*isol, biosynth*)

4-[2,2′-Bithiophen-5-yl]-3-butyn-1-ol, 9CI B-80167

Updated Entry replacing H-01421

4-[5-(2-Thienyl)-2-thienyl]-3-butyn-1-ol, 8CI. 5-(4-Hydroxy-1-butynyl)-2,2′-bithiophene

[1137-87-7]



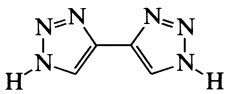
$C_{12}H_{10}OS_2$ M 234.342
Constit. of the roots of *Tagetes minuta, Echinops sphaerocephalus, Cullumia* and *Berkheya* spp. Cryst. (Et_2O/pet. ether). Mp 67° (59°).

Ac:
$C_{14}H_{12}O_2S$ M 244.314
Constit. of *T. patula, T. erecta, T. minuta, E. sphaerocephalus, C.* and *B.* spp. etc. Oil. $Bp_{0.001}$ 115°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 2945; 1964, **97**, 2125; 1965, **98**, 155, 876; 1975, **108**, 515 (*isol, uv, ir, pmr, struct, biosynth*)
Atkinson, R.E. *et al*, *J. Chem. Soc.*, 1965, 7109 (*isol*)
Bohlmann, F. *et al*, *Phytochemistry*, 1976, **15**, 1309 (*isol*)

4,4′-Bi-1*H*-1,2,3-triazole B-80168

[119720-89-7]



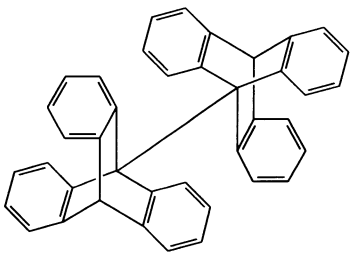
$C_4H_4N_6$ M 136.116
Cryst. (MeOH). Mp 280° dec.

Banert, K., *Chem. Ber.*, 1989, **122**, 1175 (*synth, ir, pmr, cmr*)

9,9′-Bitriptycyl B-80169

9,9′(10H,10H′)-Bi-9,10[1′,2′]benzenoanthracene, 9CI. 9,9′-Bitryptycene

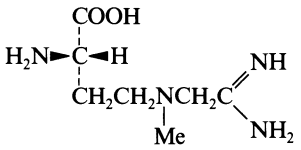
[7213-66-3]



$C_{40}H_{26}$ M 506.645
Cryst. ($PhNO_2$). Mp 577°.

Bartlett, P.D. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 1088 (*synth, ir*)
Koukotas, C. *et al*, *J. Org. Chem.*, 1966, **31**, 1970 (*synth, ir, uv, ms*)
Ardebili, M.H.P. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 7994 (*cryst struct*)

Blastidic acid B-80170



$C_7H_{16}N_4O_2$ M 188.229

(*S*)-*form*

L-form

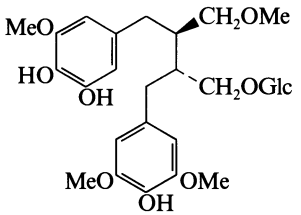
Component of Blasticidin *S*.

B,2HCl: Needles (EtOH). Mp 192-192.5° dec. $[\alpha]_D^{15}$ +25.0° (c, 1 in H_2O).

Otake, N. *et al*, *Agric. Biol. Chem.*, 1966, **30**, 126.
Yonehara, H. *et al*, *Tetrahedron Lett.*, 1966, 3785 (*abs config*)

Bonafousioside B-80171

[115900-10-2]

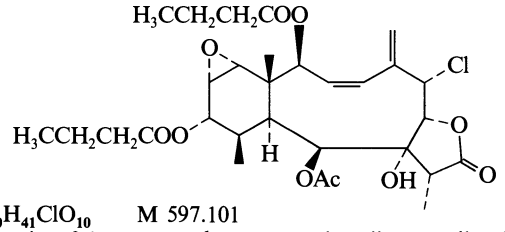


$C_{28}H_{40}O_{13}$ M 584.616

Constit. of *Bonafousia macrocalyx*.

Garnier, J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 484.

Brianthein V B-80172



$C_{30}H_{41}ClO_{10}$ M 597.101

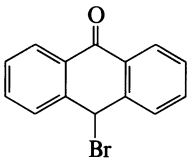
Constit. of *Briareum asbestinum*. Pale yellow needles. Mp 222°. $[\alpha]_D^{20}$ −57° (c, 1.2 in $CHCl_3$).

Coval, S.J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 981 (*isol, pmr, cmr, cryst struct*)

10-Bromoanthrone, 8CI B-80173

*10-Bromo-9(10*H*)-anthracenone, 9CI*

[1560-32-3]



$C_{14}H_9BrO$ M 273.128

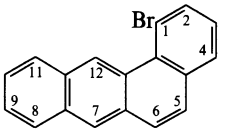
Keto-form (illus.) predominates in $CDCl_3$ soln. Yellow needles (toluene). Mp 148°.

[51678-94-5]

Meyer, K.H., *Justus Liebigs Ann. Chem.*, 1911, **379**, 37 (*synth*)
Koch, W. *et al*, *Helv. Chim. Acta*, 1965, **48**, 554 (*pmr*)
Branz, S.E. *et al*, *Synth. Commun.*, 1986, **16**, 441 (*synth, pmr, tautom*)

1-Bromobenz[*a*]anthracene, 9CI B-80174

[78302-32-6]



$C_{18}H_{11}Br$ M 307.189

Cryst. (C_6H_6). Mp 167-168°.

Hallmark, R.K., *J. Labelled Compd. Radiopharm.*, 1981, **18**, 331 (*synth*)

2-Bromobenz[*a*]anthracene, 9CI B-80175

[78302-30-4]

$C_{18}H_{11}Br$ M 307.189

Cryst. (C_6H_6). Mp 159.5-161°.

Hallmark, R.K., *J. Labelled Compd. Radiopharm.*, 1981, **18**, 331 (*synth*)
Carmichael, I. *et al*, *J. Phys. Chem. Ref. Data*, 1987, **16**, 239 (*uv*)

3-Bromobenz[*a*]anthracene, 9CI B-80176

[78302-31-5]

$C_{18}H_{11}Br$ M 307.189

Cryst. (C_6H_6). Mp 189-191°.

Hallmark, R.K., *J. Labelled Compd. Radiopharm.*, 1981, **18**, 331 (*synth*)

4-Bromobenz[*a*]anthracene, 9CI B-80177

[61921-39-9]

$C_{18}H_{11}Br$ M 307.189

Needles (C_6H_6), plates (AcOH). Mp 215-216°.

[61921-52-6]

Badger, G.M. *et al*, *J. Chem. Soc.*, 1949, 799 (*synth*)
Bodger, E.O. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 125 (*cryst struct*)
Cho, B.P. *et al*, *J. Org. Chem.*, 1987, **52**, 5668 (*synth, pmr, uv*)

7-Bromobenz[*a*]anthracene, 9CI B-80178

$C_{18}H_{11}Br$ M 307.189

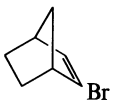
Needles or plates (AcOH), pale orange needles. Mp 150-151° (147.5-148.5°).

▷ Weak carcinogen.

Picrate: Blood-red, flat needles (AcOH). Mp 155.5-156.5°.

Badger, G.M. *et al*, *J. Chem. Soc.*, 1940, 409 (*synth*)
Mikhailov, B.M. *et al*, *Zh. Obshch. Khim.*, 1951, **21**, 2184; *ca*, **46**, 8080a (*synth*)
Yagi, H. *et al*, *J. Labelled Compd. Radiopharm.*, 1976, **12**, 127 (*synth*)
Lee, H.M. *et al*, *J. Org. Chem.*, 1979, **44**, 4948 (*synth*)

2-Bromobicyclo[2.2.1]hept-2-ene, 9CI B-80179



C_7H_9Br M 173.052

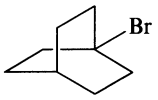
(±)-*form* [105231-24-1]

Oil. Bp_{15} 65-66°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 879 (*synth, pmr, cmr*)

1-Bromobicyclo[2.2.2]octane B-80180

[7697-09-8]

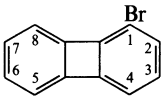


$C_8H_{13}Br$ M 189.095
Cryst. (EtOH aq. or by subl.). Mp 63.5-64.5°.

Grob, C.A. *et al*, *Helv. Chim. Acta*, 1958, **41**, 1191 (*synth*)
Suzuki, Z. *et al*, *J. Org. Chem.*, 1967, **32**, 31 (*synth*)

1-Bromobiphenylene B-80181

[17557-58-3]



$C_{12}H_7Br$ M 231.091
Pale yellow oil.

2,4,7-Trinitrofluorenone complex: [17557-57-2].
Deep red leaflets (C_6H_6/MeOH). Mp 181-183°.

Barton, J.W. *et al*, *J. Chem. Soc. C*, 1968, 28 (*synth*, *uv*)

2-Bromobiphenylene B-80182

[17573-59-0]

$C_{12}H_7Br$ M 231.091
Pale yellow plates (MeOH). Mp 64-65°.

2,4,7-Trinitrofluorenone complex: Scarlet needles (EtOH/AcOH). Mp 136-137°.

Baker, W. *et al*, *J. Chem. Soc.*, 1958, 2658, 2666 (*synth*, *uv*)
Blatchly, J.M. *et al*, *J. Chem. Soc. C*, 1969, 2789 (*pmr*)
McKillop, A. *et al*, *J. Org. Chem.*, 1972, **37**, 88 (*synth*)
Cracknell, M.E. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1985, 115 (*synth*)

Bromocarbonimidic difluoride B-80183

N-*Bromo-1,1-difluoromethanimine*, *9CI*

$F_2C{=}NBr$

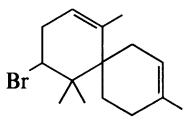
$CBrF_2N$ M 110.913
Pale yellow gas. Mp −93° to −92°. Bp 14.5°.

O'Brien, B.A. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 4266 (*synth*, *ir*, *raman*, *F*-19 *nmr*, *uv*)
Bauknight, C.W. *et al*, *J. Org. Chem.*, 1988, **53**, 4443 (*synth*)

10-Bromo-2,7-chamigradiene B-80184

10-Bromo-α-chamigrene

[57473-87-7]

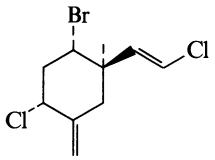


$C_{15}H_{23}Br$ M 283.251
Metab. of *Laurencia pacifica*. Oil. $[\alpha]_D$ −71.1° (c, 0.18 in $CHCl_3$).

Havard, B.M. *et al*, *Tetrahedron Lett.*, 1976, 2519.

2-Bromo-4-chloro-1-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane, 9CI B-80185

[119903-45-6]



$C_{10}H_{13}BrCl_2$ M 284.022
Constit. of *Plocamium hamatum*. Oil. $[\alpha]_D$ −34° (c, 0.008 in $CHCl_3$).

Coll, J.C. *et al*, *Aust. J. Chem.*, 1988, **41**, 1743.

1-Bromo-2-chloro-1,1,2-trifluoroethane, 9CI B-80186

[354-06-3]

$F_2CBrCHFCl$

$C_2HBrClF_3$ M 197.382
Inhalation anaesthetic agent. d_4^{25} 1.864. Bp 50-55°, Bp_{615} 46.02°. n_D^{20} 1.3705, n_D^{25} 1.3685.

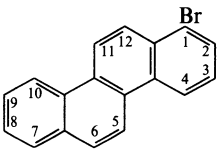
▷ Irritant.

[74925-63-6]

Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1954, 3747 (*synth*)
Lee, J. *et al*, *Trans. Faraday Soc.*, 1958, **54**, 308 (*F*-19 *nmr*, *pmr*)
Kakac, B. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 745 (*ir*)
Norris, R.D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 182 (*F*-19 *nmr*)
Ng, S., *J. Magn. Reson.*, 1975, **17**, 244 (*pmr*)
Kirk-Othmer Encycl. Chem. Technol., 3*rd Ed.*, 1978-1984, *Wiley, NY*, 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 258; **10**, 868 (*props*)
Cascorbi, H.F. *et al*, *Anaesthesist*, 1980, **29**, 169 (*tox*, *use*)

1-Bromochrysene B-80187

[76670-38-7]



$C_{18}H_{11}Br$ M 307.189
Cryst. (C_6H_6). Mp 240-241°.

Archer, W.J. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 2, 1980, 1828 (*synth*, *pmr*)

2-Bromochrysene B-80188

[55120-48-4]

$C_{18}H_{11}Br$ M 307.189
Photosensitizer. Silvery plates ($CHCl_3$). Mp 261-262°. A 1966 ref. referring to 2-bromochrysene was incorr. numbered and in fact referred to 6-bromochrysene.

Archer, W.J. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 2, 1980, 1828 (*synth*, *pmr*)

3-Bromochrysene B-80189

[56158-60-2]

$C_{18}H_{11}Br$ M 307.189
Cryst. (Me_2CO). Mp 182.5-183° (195-196°).

Masetti, F. *et al*, *Gazz. Chim. Ital.*, 1975, **105**, 419 (*synth*, *props*)
Archer, W.J. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 2, 1980, 1828 (*synth*, *pmr*)

4-Bromochrysene **B-80190**

[76670-41-2]

$C_{18}H_{11}Br$ M 307.189
Oil.

Archer, W.J. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1980, 1828 (*synth*)

5-Bromochrysene **B-80191**

$C_{18}H_{11}Br$ M 307.189
Fine needles (EtOH). Mp 98°.

Archer, W.J. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1980, 1828 (*synth, pmr*)

6-Bromochrysene **B-80192**

[7397-93-5]

$C_{18}H_{11}Br$ M 307.189
The 1966 paper incorr. reports this as 2-bromochrysene.
Cryst. (C_6H_6). Mp 153.6-155°.

Altschuler, L. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 5837 (*synth*)
Archer, W.J. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1980, 1828 (*synth, pmr*)
Van Bladeren, P.J. *et al*, *Tetrahedron Lett.*, 1983, **24**, 4903 (*synth, pmr*)
Cho, B.P. *et al*, *J. Org. Chem.*, 1987, **52**, 5668 (*synth, pmr, ms, chromatog*)

2-Bromo-1,2-dichloro-1,1-difluoroethane, 9CI **B-80193**

[2821-90-1]

$F_2CClCHBrCl$

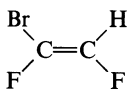
$C_2HBrCl_2F_2$ M 213.836

(±)-***form***
Shows anaesthetic props. Bp 95.5°, Bp 76-78°. n_D^{20} 1.4298.

Di Paola, T. *et al*, *J. Pharm. Sci.*, 1979, **68**, 39 (*pharmacol*)
Caphiel, P. *et al*, *Tetrahedron*, 1979, **35**, 2661 (*synth, pmr, F nmr*)

1-Bromo-1,2-difluoroethylene, 8CI **B-80194**

1-Bromo-1,2-difluoroethene, 9CI



(*E*)-*form*

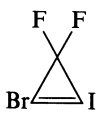
C_2HBrF_2 M 142.931

(***E***)-***form***
cis-form
Gas. Bp 16°.

(***Z***)-***form*** [3685-10-7]
trans-form
Gas. Bp 13°.

Demiel, A., *J. Org. Chem.*, 1965, **30**, 2121 (*synth, pmr, F nmr, ir*)

1-Bromo-3,3-difluoro-2-iodocyclopropene, 9CI **B-80195**



C_3BrF_2I M 280.838
Liq., isol. by glc. n_D^{27} 1.5326.

Sepiol, J. *et al*, *J. Org. Chem.*, 1975, **40**, 3791 (*synth, ir, F-19 nmr*)

1-Bromo-1,1-difluoro-2-iodoethane, 9CI **B-80196**

[420-93-9]

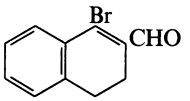
F_2CBrCH_2I

$C_2H_2BrF_2I$ M 270.843
Bp_{216} 84°. n_D^{20} 1.504.

Haszeldine, R.N., *J. Chem. Soc.*, 1953, 1764; 1954, 923 (*synth, uv*)

1-Bromo-3,4-dihydro-2-naphthalenecarboxaldehyde, 9CI **B-80197**

[117582-62-4]



$C_{11}H_9BrO$ M 237.095
Yellow solid (EtOH). Mp 42-44°.

Gilchrist, T.L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2595 (*synth, ir, pmr, ms*)

2-Bromo-3,4-dihydro-1-naphthalenecarboxaldehyde, 9CI **B-80198**

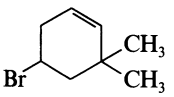
[112631-07-9]

$C_{11}H_9BrO$ M 237.095
Mp 26-27°.

Ethylene acetal:
$C_{13}H_{13}BrO_2$ M 281.148
Cryst. (Et_2O/pet. ether). Mp 62-63°.

Gilchrist, T.L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2595 (*synth, ir, pmr, ms*)

5-Bromo-3,3-dimethylcyclohexene **B-80199**



$C_8H_{13}Br$ M 189.095

(±)-***form*** [113647-43-1]
Liq. Bp_{26} 90-92°.

McIntosh, J.M. *et al*, *J. Org. Chem.*, 1988, **53**, 1947 (*synth, pmr*)

3-Bromo-2,2-dimethylpropanol **B-80200**

[40894-00-6]

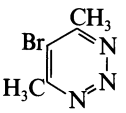
$BrCH_2C(CH_3)_2CH_2OH$

$C_5H_{11}BrO$ M 167.045
Bp_{13} 80°.

Searles, S. *et al*, *J. Org. Chem.*, 1960, **24**, 1839 (*synth*)
Hua, D.Y. *et al*, *J. Org. Chem.*, 1988, **53**, 507 (*synth, ir, pmr*)

5-Bromo-4,6-dimethyl-1,2,3-triazine **B-80201**

[109520-03-8]



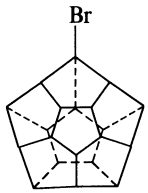
$C_5H_6BrN_3$ M 188.026
Needles (hexane). Mp 104-105°.

Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

Bromododecahedrane B-80202

*1-Bromohexadecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene, 9CI*

[112896-27-2]

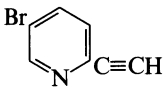


$C_{20}H_{19}Br$ M 339.274
Solid. Mp >240°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **53**, 1303 (*synth, cmr*)

5-Bromo-2-ethynylpyridine B-80203

[111770-86-6]

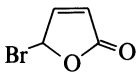


C_7H_4BrN M 182.019
Cryst. by subl. Mp 84-86°.

Tilley, J.W. *et al*, *J. Org. Chem.*, 1988, **53**, 386 (*synth, ms, pmr*)

5-Bromo-2(5*H*)-furanone, 9CI B-80204

[40125-53-9]



$C_4H_3BrO_2$ M 162.970

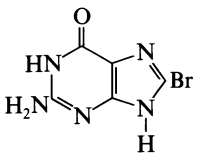
(±)-*form*
$Bp_{0.1}$ 69-70°.

Elming, N. *et al*, *Acta Chem. Scand.*, 1952, **6**, 565 (*synth*)
Doerr, I.L. *et al*, *J. Org. Chem.*, 1973, **38**, 3878 (*synth, ir, pmr*)
Wolff, S. *et al*, *Synthesis*, 1988, 760 (*synth*)

8-Bromoguanine, 8CI B-80205

*2-Amino-8-bromo-1,7-dihydro-6*H*-purin-6-one, 9CI. 2-Amino-8-bromo-6-hydroxypurine*

[3066-84-0]



$C_5H_4BrN_5O$ M 230.023
Cryst. (H_2O). Insol. H_2O, EtOH, Et_2O.

Fischer, E. *et al*, *Justus Liebigs Ann. Chem.*, 1883, **221**, 336 (*synth*)
Holmes, R.E. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1242 (*synth*)

1-Bromo-1,1,2,2,3,3,3-heptafluoropropane, 9CI B-80206

Heptafluoropropyl bromide. Perfluoropropyl bromide. Heptafluorobromopropane

[422-85-5]

$F_3CCF_2CF_2Br$

C_3BrF_7 M 248.926
d_4^0 1.87. Bp_{742} 15-15.2°, Bp 11-13°. $n_D^{-42.2}$ 1.3131, $n_D^{-29.8}$ 1.3070.

▷ Irritant.

Hauptschein, M. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 1347 (*synth, ir*)
Nodiff, E.A. *et al*, *J. Org. Chem.*, 1953, **18**, 235 (*ir, props*)
Husted, D.R. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 5141 (*synth, ir*)
Evans, D.F. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 238 (*F*-19 *nmr*)

2-Bromo-1,1,1,2,3,3,3-heptafluoropropane, 9CI B-80207

[422-77-5]

$F_3CCFBrCF_3$

C_3BrF_7 M 248.926
Mobile liq. Bp 15-16° (11-12°) .

Barlow, G.B. *et al*, *J. Chem. Soc.*, 1955, 1749 (*synth*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Eujen, R. *et al*, *J. Fluorine Chem.*, 1983, **22**, 263 (*F*-19 *nmr*)

6-Bromo-1-heptene B-80208

[38334-98-4]

$H_2C{=}CH(CH_2)_3CHBrCH_3$

$C_7H_{13}Br$ M 177.084

(±)-*form*
Liq. Bp_{17} 59-61°.

Ashby, E.C. *et al*, *J. Org. Chem.*, 1988, **53**, 6068 (*synth, pmr, ms*)

1-Bromo-3-hexene, 9CI B-80209

$H_3CCH_2CH{=}CHCH_2CH_2Br$

$C_6H_{11}Br$ M 163.057

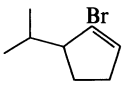
(*E*)-*form* [63281-96-9]
Liq. Bp_{15} 78-80°.

(*Z*)-*form* [5009-31-4]
Liq. Bp 149-151°, Bp_{15} 65°.

Harper, S.H. *et al*, *J. Chem. Soc.*, 1955, 1512 (*synth*)
Stetter, H. *et al*, *Synthesis*, 1975, 379 (*synth*)
Sun, P.E. *et al*, *Can. J. Chem.*, 1979, **57**, 1475 (*synth, ir, pmr, ms*)
Rao, A.V.R. *et al*, *Tetrahedron*, 1987, **43**, 4385 (*synth, pmr*)

1-Bromo-5-isopropylcyclopentene B-80210

1-Bromo-5-(1-methylethyl)cyclopentene, 9CI



$C_8H_{13}Br$ M 189.095

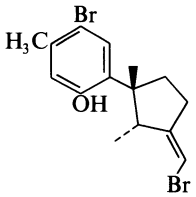
(±)-*form* [112655-69-3]
Liq. Bp_7 68-69°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 890 (*synth, pmr, cmr*)

9-Bromolaurenisol B-80211

Updated Entry replacing B-02636

[72782-83-3]



$C_{15}H_{18}Br_2O$ M 374.115

Constit. of *Laurencia glandulifera*. Oil. $[\alpha]_D^{22}$ +74° (c, 0.6 in $CHCl_3$).

Suzuki, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 3349 (*isol*)
Capon, R.J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1302 (*isol*, *pmr*)

Bromomethanol B-80212

[50398-29-3]

$BrCH_2OH$

CH_3BrO M 110.938

Ac: [590-97-6].
$C_3H_5BrO_2$ M 152.975
Alkylating agent. Oil. Bp 132-138°.

Chloroacetyl:
$C_3H_4BrClO_2$ M 187.420
Oil. d_4^{20} 1.783. $Bp_{3.5}$ 57.2°. n_D^{20} 1.4873.

Benzoyl: [40796-19-8].
$C_8H_7BrO_2$ M 215.046
Oil. Bp_{19} 135-137°, $Bp_{0.3}$ 62-65°.

4-Methylbenzenesulfonyl: [117184-51-7].
$C_8H_9BrO_3S$ M 265.127
Oil or low melting solid, may be recryst. from MeOH at 0-5°. Mp <20°. $Bp_{0.4}$ 112-114°.

Ulich, L.H. *et al*, *J. Am. Chem. Soc.*, 1921, **43**, 660 (*acetate*)
Euranto, E.K. *et al*, *Acta Chem. Scand.*, 1966, **20**, 1273 (*chloroacetate*)
Bodor, N. *et al*, *J. Med. Chem.*, 1980, **23**, 566 (*benzoate*, *synth*, *ir*, *pmr*)
Hahn, R.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5783 (*tosylate*, *synth*, *pmr*, *cmr*)

3-Bromo-3-methyl-1-butyne B-80213

[6214-31-9]

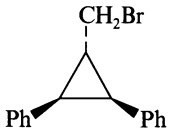
$(H_3C)_2CBrC{\equiv}CH$

C_5H_7Br M 147.014
d_4^{25} 1.268. Bp_{106} 42.2°. n_D^{25} 1.4118.

Shiner, V.J. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 2402.
Jacobs, T.L. *et al*, *J. Org. Chem.*, 1963, **28**, 1360 (*synth*, *ir*)

1-Bromomethyl-2,3-diphenylcyclopropane B-80214

1,1'-[3-(Bromomethyl)-1,2-cyclopropanediyl]bisbenzene, 9CI



$C_{16}H_{15}Br$ M 287.198

(1α,2β,3β)-form [117021-83-7]

Cryst. (pet. ether). Mp 58.0-58.5°.

Castellino, A.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 7512 (*synth*, *pmr*)

1-(Bromomethyl)-2-fluorobenzene, 9CI B-80215

α-Bromo-o-fluorotoluene, 8CI. o-Fluorobenzyl bromide

[446-48-0]

C_7H_6BrF M 189.027

Liq. Bp 195-202°, Bp_{15} 86-87°.

▷ Corrosive, lachrymator.

Olah, G. *et al*, *J. Org. Chem.*, 1957, **22**, 879 (*synth*)
Bergman, E.D. *et al*, *Tetrahedron*, 1976, **32**, 2847 (*props*)

1-(Bromomethyl)-3-fluorobenzene, 9CI B-80216

α-Bromo-m-fluorotoluene, 8CI. m-Fluorobenzyl bromide

[456-41-7]

C_7H_6BrF M 189.027

Bp 196-200°, Bp_{15} 84-85°.

▷ Corrosive, lachrymator.

Olah, G. *et al*, *J. Org. Chem.*, 1957, **22**, 879 (*synth*)
Tait, J.M.S. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 4 (*ms*)
Roberts, B.P. *et al*, *J. Chem. Soc.*, *Chem. Commun.*, 1978, 752 (*synth*)
Happer, D.A.R. *et al*, *Org. Magn. Reson.*, 1983, **21**, 252 (*F-nmr*)

1-(Bromomethyl)-4-fluorobenzene, 9CI B-80217

α-Bromo-p-fluorotoluene, 8CI. p-Fluorobenzyl bromide

[459-46-1]

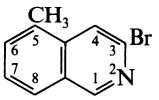
C_7H_6BrF M 189.027

Bp_{27} 92-102°. n_D 1.547.

▷ Corrosive, lachrymator.

Olah, G. *et al*, *J. Org. Chem.*, 1957, **22**, 879 (*synth*)
Tait, J.M.S. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 4 (*ms*)
Verdonck, L. *et al*, *Spectrochim. Acta*, *Part A*, 1972, **28**, 55 (*ir*, *raman*)
Roberts, B.P. *et al*, *J. Chem. Soc.*, *Chem. Commun.*, 1978, 752 (*synth*)
Happer, D.A.R. *et al*, *Org. Magn. Reson.*, 1983, **21**, 252 (*F nmr*)

3-Bromo-5-methylisoquinoline, 9CI B-80218



$C_{10}H_8BrN$ M 222.084

Cryst. (C_6H_6/hexane). Mp 90-91°.

Ban, Y. *et al*, *Chem. Pharm. Bull.*, 1964, **12**, 1296 (*synth*)

4-Bromo-1-methylisoquinoline, 9CI B-80219

[104704-40-7]

$C_{10}H_8BrN$ M 222.084

Needles (hexane). Mp 48-49°.

Sawanishi, H. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 4564 (*synth*, *pmr*)

5-Bromo-3-methylisoquinoline, 9CI B-80220

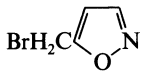
[16552-67-3]

$C_{10}H_8BrN$ M 222.084
Cryst. Mp 40-42°. $Bp_{0.75}$ 35° subl.

Hamilton, H.J., *J. Heterocycl. Chem.*, 1967, **4**, 410 (*synth*)

5-(Bromomethyl)isoxazole B-80221

[69735-35-9]



C_4H_4BrNO M 161.986
Liq. $Bp_{0.5}$ 58-62°.

DeShong, P. *et al*, *J. Org. Chem.*, 1988, **53**, 1356 (*synth, ir, pmr, ms*)

(Bromomethyl)pentafluorobenzene, 9CI B-80222

Pentafluorobenzyl bromide

[1765-40-8]

$(C_6F_5)CH_2Br$

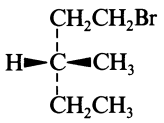
$C_7H_2BrF_5$ M 260.989
Liq. Bp 174-175°.

▷ Extremely lachrymatory.

Barbour, A.K. *et al*, *J. Chem. Soc.*, 1961, 808 (*synth, ir*)

1-Bromo-3-methylpentane B-80223

[51116-73-5]



$C_6H_{13}Br$ M 165.073

(R)-form

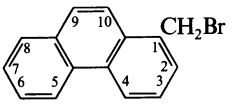
Oil. Bp_{63} 71-72.5°. $[\alpha]_D^{20}$ −19.43° (neat).

[22299-70-3]

Mori, K. *et al*, *Tetrahedron*, 1984, **40**, 299 (*synth, ir, pmr*)
Fuganti, C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3061 (*synth*)

1-(Bromomethyl)phenanthrene, 9CI B-80224

[42050-05-5]



$C_{15}H_{11}Br$ M 271.156
Leaflets (C_6H_6/pet. ether). Mp 97°.

Bachmann, W.E. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 2207 (*synth*)

2-(Bromomethyl)phenanthrene B-80225

[2417-66-5]

$C_{15}H_{11}Br$ M 271.156
Needles (C_6H_6). Mp 111-111.5°.

Mosettig, E. *et al*, *J. Am. Chem. Soc.*, 1933, **55**, 2995 (*synth*)

3-(Bromomethyl)phenanthrene B-80226

[24471-44-1]

$C_{15}H_{11}Br$ M 271.156
Needles (C_6H_6). Mp 117.5° (114.5-115°).

Mosettig, E. *et al*, *J. Am. Chem. Soc.*, 1933, **55**, 2995 (*synth*)
Bachmann, W.E. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 2207 (*synth*)

9-(Bromomethyl)phenanthrene B-80227

[24471-57-6]

$C_{15}H_{11}Br$ M 271.156
Cryst. Mp 118.5-119° (103-103.5°).

Mosettig, E. *et al*, *J. Am. Chem. Soc.*, 1933, **55**, 2995 (*synth*)
Bachmann, W.E. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 2207 (*synth*)
Lambert, J.B. *et al*, *J. Org. Chem.*, 1979, **44**, 1480 (*synth, ir, pmr*)
Sugimoto, A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2579 (*synth, pmr, ms*)

1-Bromo-2-methyl-1-phenylpropene B-80228

(1-Bromo-2-methyl-1-propenyl)benzene

$(H_3C)_2C{=}CBrPh$

$C_{10}H_{11}Br$ M 211.101
Liq. $Bp_{0.8}$ 90-100° (Kugelrohr) .

Maloney, M.G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2847 (*synth, uv, pmr*)

2-Bromo-2-methylpropanoic acid, 9CI B-80229

Updated Entry replacing B-02834

2-Bromoisobutyric acid

[2052-01-9]

$(H_3C)_2CBrCOOH$

$C_4H_7BrO_2$ M 167.002
Cryst. Mp 48-49°. Bp 198-200°, Bp_{20} 115°.

Me ester: [23426-63-3].
$C_5H_9BrO_2$ M 181.029
Liq. Bp_9 38°, Bp_{19} 51-52°.

Bromide: [20769-85-1].
$C_4H_6Br_2O$ M 229.899
Liq. Bp 162-164°, Bp_{100} 91-98°.

Anhydride: [42069-15-8].
$C_8H_{12}Br_2O_3$ M 315.989
Cryst. Mp 63-65°. Bp_{35} 135-140°.

Amide: [7462-74-0].
C_4H_8BrNO M 166.017
Cryst. Mp 148°. Bp_{17} 145°.

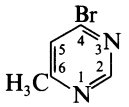
Anilide:
$C_{10}H_{12}BrNO$ M 242.115
Cryst. (EtOH aq.). Mp 83°.

Nitrile: [41658-69-9]. *α-Bromoisobutyronitrile. 2-Bromo-2-cyanopropane*
C_4H_6BrN M 148.002
Liq. d_4^{25} 1.38. Bp 137-139°.

Michael, A., *Ber.*, 1901, **34**, 4043 (*synth*)
Stevens, C.L., *J. Am. Chem. Soc.*, 1948, **70**, 165 (*nitrile*)
Ford, M.C. *et al*, *J. Chem. Soc.*, 1951, 1851 (*ester*)
Org. Synth., 1953, **33**, 29 (*bromide*)
Smissman, E., *J. Am. Chem. Soc.*, 1954, **76**, 5805 (*amide*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 434.

4-Bromo-6-methylpyrimidine, 9CI B-80230

[69543-98-2]



$C_5H_5BrN_2$ M 173.012
Mp 29-31°. Bp_{18} 105-110°. Slowly dec. on standing.

Rasmussen, C.A.H. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1979, **98**, 5 (*synth*)

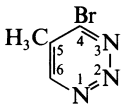
5-Bromo-4-methylpyrimidine, 9CI B-80231

[1439-09-4]

$C_5H_5BrN_2$ M 173.012
Liq. Bp_{23} 90°, Bp_{14} 72-73°.

van der Plas, H.C., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1965, **84**, 1101 (*synth*)
Geerts, J. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1974, **93**, 231 (*pmr*)
Yamenaka, H. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 3119 (*synth*, *pmr*)

4-Bromo-5-methyl-1,2,3-triazine B-80232



$C_4H_4BrN_3$ M 174.000
Needles (hexane). Mp 36-38°. Subl. very readily.

Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth*, *pmr*)

5-Bromo-4-methyl-1,2,3-triazine B-80233

[114078-90-9]

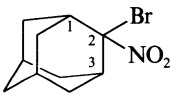
$C_4H_4BrN_3$ M 174.000
Needles (hexane). Mp 73-74°.

Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth*, *pmr*)

2-Bromo-2-nitroadamantane B-80234

2-Bromo-2-nitrotricyclo[3.3.1.1^{3,7}]decane

[40854-02-2]



$C_{10}H_{14}BrNO_2$ M 260.130
Cryst. (EtOH aq.). Mp 190-191°.

Archibald, T.G. *et al*, *J. Org. Chem.*, 1988, **53**, 4645 (*synth*, *ir*, *pmr*)

4-Bromo-2-nitrobenzaldehyde, 9CI B-80235

Updated Entry replacing B-02967

[5551-12-2]

$C_7H_4BrNO_3$ M 230.017
Yellow cryst. (EtOH). Mp 97-98°.

Oxime:
$C_7H_5BrN_2O_3$ M 245.032
Mp 164°.

Semicarbazone: Cryst. (AcOH). Mp 276° (270-272°).

Phenylhydrazone: Brown-red cryst. Mp 181-182°.

Sachs, F. *et al*, *Ber.*, 1904, **37**, 1861 (*synth*)
Barber, H.J. *et al*, *J. Chem. Soc.*, 1945, 167 (*synth*)
Dandegaonker, S.H., *CA*, 1966, **64**, 17463; *J. Indian Chem. Soc.*, 1969, **46**, 148 (*synth*, *uv*)
Danieli, R. *et al*, *CA*, 1968, **69**, 106403 (*synth*)
Voss, G. *et al*, *Chem. Ber.*, 1989, **122**, 1199 (*synth*, *uv*, *pmr*, *cmr*, *ms*)

4-Bromo-3-nitrobenzaldehyde, 9CI B-80236

Updated Entry replacing B-02968

$C_7H_4BrNO_3$ M 230.017
Pale-yellow needles (EtOH). Mp 106°. Steam-volatile.

Oxime:
$C_7H_5BrN_2O_3$ M 245.032
Orange-yellow needles (EtOH). Mp 154°.

p-*Nitrophenylhydrazone:* Yellow needles. Mp 282-283°.

Semicarbazone: Mp 254-255° dec.

Phenylhydrazone: Two forms: red and yellow. Mp 146-147° (both forms).

Hodgson, H.H. *et al*, *J. Chem. Soc.*, 1927, 20 (*synth*)
Voss, G. *et al*, *Chem. Ber.*, 1989, **122**, 1199 (*uv*, *pmr*, *cmr*, *ms*)

5-Bromo-2-nitrobenzaldehyde, 9CI B-80237

Updated Entry replacing B-02969

[20357-20-4]

$C_7H_4BrNO_3$ M 230.017
Cryst. (C_6H_6 or EtOH aq.) or needles (C_6H_6/cyclohexane). Mp 77-78°.

▷ CU4875000.

Oxime:
$C_7H_5BrN_2O_3$ M 245.032
Yellow needles. Mp 113°.

Phenylhydrazone: Red needles (EtOH). Mp 180° dec.

Mettler, C., *Ber.*, 1905, **38**, 2809.
Alford, E.J. *et al*, *J. Chem. Soc.*, 1952, 2102.
Danieli, R. *et al*, *CA*, 1968, **69**, 106403 (*synth*)
Voss, G. *et al*, *Chem. Ber.*, 1989, **122**, 1199 (*synth*, *uv*, *pmr*, *cmr*, *ms*)

4-Bromo-2-nitrobenzyl alcohol, 8CI B-80238

4-Bromo-2-nitrobenzenemethanol, 9CI

[22996-19-6]

$C_7H_6BrNO_3$ M 232.033
Needles (EtOH). Mp 80-81°.

Cal'bershtam, M. *et al*, *Zh. Org. Khim.*, 1969, **5**, 953; *jocet*, 1969, 938 (*synth*, *ir*)

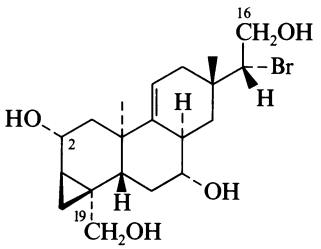
2-Bromo-4-nitrothiophene B-80239

[81975-00-0]

$C_4H_2BrNO_2S$ M 208.035
Liq. Bp_{55} 105-110°, $Bp_{0.6}$ 64-68°.

Elliott, R.L. *et al*, *Tetrahedron*, 1987, **43**, 3295 (*synth*, *ir*, *pmr*)

15-Bromo-9(11)-parguerene-2,7,16,19-tetrol B-80240



$C_{20}H_{31}BrO_4$ M 415.366

(2α,7α)-form

2-Ac: [83115-36-0]. *2α-Acetoxy-15-bromo-9(11)-parguerene-7α,16,19-triol.* ***Parguerene***
$C_{22}H_{33}BrO_5$ M 457.404
Metab. of *Aplysia dactylomela*. Oil. $[\alpha]_D$ −40° (c, 0.03 in $CHCl_3$).

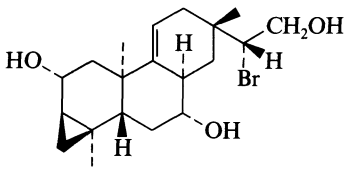
19-Deoxy, 2-Ac: [83115-44-0]. *2α-Acetoxy-15-bromo-9(11)-parguerene-7α,16-diol.* ***Deoxyparguerene***
$C_{22}H_{33}BrO_4$ M 441.404
Metab. of *A. dactylomela*. Oil. $[\alpha]_D$ −35.8° (c, 0.62 $CHCl_3$).

19-Deoxy, 2,16-di-Ac: [82668-11-9]. *2α,16-Diacetoxy-15-bromo-9(11)-pargueren-7α-ol*
$C_{24}H_{35}BrO_5$ M 483.441
Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D$ −48° (c, 0.1 in MeOH).

Schmitz, F.J. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 6415 (*isol*)
Higgs, M.D. *et al*, *Phytochemistry*, 1982, **21**, 789 (*isol*)
Suzuki, T. *et al*, *Chem. Lett.*, 1989, 969 (*deriv*)

15-Bromo-9(11)-parguerene-2,7,16-triol B-80241

15-Bromo-2,7,16-trihydroxy-9(11)-parguerene



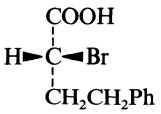
Absolute configuration

$C_{20}H_{31}BrO_3$ M 399.367
Metab. of *Laurencia obtusa*. Cryst. Mp 173-174°. $[\alpha]_D$ −36.4° (c, 1.85 in $CHCl_3$).

Suzuki, T. *et al*, *Chem. Lett.*, 1989, 969 (*cryst struct*)

2-Bromo-4-phenylbutanoic acid, 9CI B-80242

Updated Entry replacing B-03154
[16503-46-1]



(*R*)-*form*

$C_{10}H_{11}BrO_2$ M 243.100

(R)-form
Oil. $[\alpha]_D^{20}$ +65.5° (c, 1 in $CHCl_3$).

Et ester:
$C_{12}H_{15}BrO_2$ M 271.153
Oil. $[\alpha]_D^{20}$ +55° (c, 1 in $CHCl_3$).

(±)-form
Oil. d_4^{25} 1.44. Bp_1 145-147°.

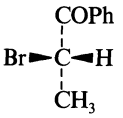
Et ester: Yellow liq. Bp_{14} 157°.

Amide:
$C_{10}H_{12}BrNO$ M 242.115
Cryst. (EtOAc). Mp 130-131°.

Fischer, E. *et al*, *Ber.*, 1906, **39**, 2213 (*synth*)
v. Braun, J., *Ber.*, 1923, **56**, 2178 (*ester*)
Stevens, C.A. *et al*, *J. Org. Chem.*, 1953, **18**, 1112 (*synth*)
Iwasaki, G. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 280 (*synth, pmr*)

2-Bromo-1-phenyl-1-propanone, 9CI B-80243

Updated Entry replacing B-03198
2-Bromopropiophenone, 8CI. 1-Bromoethyl phenyl ketone. 1-Benzoyl-1-bromoethane
[2114-00-3]



(*S*)-*form*

C_9H_9BrO M 213.073
▷ UG8400000.

(S)-form
Oil.

(±)-form
Liq. d_0^0 1.454. Bp 245-250°, Bp_{10} 125-130°. n_D^{25} 1.5686.

2,4-Dinitrophenylhydrazone: Mp 160-161°.

Bauer, D.P. *et al*, *J. Org. Chem.*, 1975, **40**, 1990 (*synth*)
Castaldi, G. *et al*, *Synthesis*, 1987, 1039 (*synth, resoln, uv, cd, pmr*)

3-Bromo-3-phenyl-1-propyne B-80244

(1-Bromo-2-propynyl)benzene, 9CI
[50874-14-1]

PhCHBrC≡CH

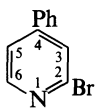
C_9H_7Br M 195.058

(±)-form
$Bp_{0.003}$ 51-53°.

Kirmse, W. *et al*, *Chem. Ber.*, 1973, **106**, 3086.
Brooks, J.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 2588.

2-Bromo-4-phenylpyridine, 9CI, 8CI B-80245

[54151-74-5]



$C_{11}H_8BrN$ M 234.095
Cryst. (pet. ether). Mp 65-66°.

Case, F.H. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 5842.

2-Bromo-5-phenylpyridine, 9CI, 8CI B-80246

[107351-82-6]
$C_{11}H_8BrN$ M 234.095
Cryst. (hexane). Mp 78-79°.

Tilley, J.W. *et al*, *J. Org. Chem.*, 1988, **53**, 386 (*synth, ms, pmr*)

2-Bromo-6-phenylpyridine, 9CI, 8CI B-80247

[39774-26-0]
$C_{11}H_8BrN$ M 234.095
Cryst. (pet. ether). Mp 51-52°.

Case, F.H. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 5842.

3-Bromo-2-phenylpyridine, 9CI, 8CI B-80248

$C_{11}H_8BrN$ M 234.095
Pale yellow liq. Bp_{720} 305-307°.

Abramovitch, R.A. *et al*, *Can. J. Chem.*, 1963, **41**, 1752 (*synth, ir*)

3-Bromo-4-phenylpyridine, 9CI, 8CI B-80249

[88345-89-5]

$C_{11}H_8BrN$ M 234.095

Cryst. Mp 49-50°.

Comins, D.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1239 (*synth, pmr*)

4-Bromo-2-phenylpyridine, 9CI, 8CI B-80250

[98420-98-5]

$C_{11}H_8BrN$ M 234.095

Oil.

Picrate: Cryst. Mp 174.5-176°.

Comins, D.L. *et al*, *J. Org. Chem.*, 1985, **50**, 4410 (*synth, ir, pmr*)

5-Bromo-2-phenylpyridine, 9CI, 8CI B-80251

[27012-25-5]

$C_{11}H_8BrN$ M 234.095

Cryst. (hexane). Mp 74-76°.

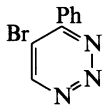
Giam, C.S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 478 (*synth*)

Comins, D.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1239 (*synth, pmr*)

Tilley, J.W. *et al*, *J. Org. Chem.*, 1988, **53**, 386 (*synth*)

5-Bromo-4-phenyl-1,2,3-triazine B-80252

[114078-92-1]



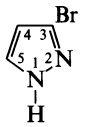
$C_9H_6BrN_3$ M 236.070

Flakes (hexane/Et_2O). Mp 125-126° dec.

Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

3(5)-Bromopyrazole, 9CI B-80253

[14521-80-3]



$C_3H_3BrN_2$ M 146.974

Cryst. by subl. Mp 70° (66°). $Bp_{0.1}$ 70-72°.

1H-form

1-Ph: [50877-46-8].

$C_9H_7BrN_2$ M 223.072

No Mp reported.

2H-form

2-Ph: [17635-42-6]. *5-Bromo-1-phenylpyrazole, 9CI*

$C_9H_7BrN_2$ M 223.072

Cryst. (EtOH aq.). Mp 56°.

Reimlinger, H.K. *et al*, *Chem. Ber.*, 1966, **99**, 3350 (*synth*)

Begtrup, M., *Acta Chem. Scand.*, 1973, **27**, 2051 (*derivs*)

Freche, P. *et al*, *Tetrahedron*, 1977, **33**, 2069 (*synth, pmr*)

Birkofer, L. *et al*, *Chem. Ber.*, 1981, **114**, 2293 (*synth, ir, pmr*)

Van Tilborg, M.W.E.M. *et al*, *Org. Mass Spectrom.*, 1984, **19**, 569 (*ms*)

4-Bromopyrazole, 9CI B-80254

[2075-45-8]

$C_3H_3BrN_2$ M 146.974

Alcohol dehydrogenase inhibitor. Cryst. by subl. Mp 91-92°.

▷ Possibly mutagenic.

1-Me: [15803-02-8]. *4-Bromo-1-methylpyrazole, 9CI*

$C_4H_5BrN_2$ M 161.001

Oily liq. Bp_{18} 76-78°. n_D^{23} 1.5298.

▷ Possibly mutagenic.

1-Ph: [15115-52-3].

$C_9H_7BrN_2$ M 223.072

Needles (EtOH). Mp 83°.

Hüttel, R. *et al*, *Justus Liebigs Ann. Chem.*, 1955, **593**, 179 (*synth, deriv*)

Elguero, J. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2832, 3727, 3744 (*synth, pmr, uv, deriv*)

Liljefors, S. *et al*, *Chem. Scr.*, 1980, **15**, 102 (*deriv*)

Claramunt, R.M. *et al*, *Bull. Soc. Chim. Fr., Part II*, 1983, 5 (*synth, cmr, pmr, deriv*)

Cabildo, P. *et al*, *Org. Magn. Reson.*, 1984, **22**, 603 (*cmr*)

Van Tilborg, M.W.E.M. *et al*, *Org. Mass Spectrom.*, 1984, **19**, 569 (*ms*)

5-Bromo-2(1*H*)-pyridinethione, 9CI B-80255

Updated Entry replacing B-60317

5-Bromo-2-pyridinethiol. 5-Bromo-2-mercaptopyridine

[56673-34-8]

C_5H_4BrNS M 190.063

S-*Me:* [51933-78-9]. *5-Bromo-2-(methylthio)pyridine*

C_6H_6BrNS M 204.090

Mp 38-39°.

S-*Me*, S-*dioxide:* [98626-95-0]. *5-Bromo-2-(methylsulfonyl)pyridine, 9CI*

$C_6H_6BrNO_2S$ M 236.089

Mp 95-96°.

U.K. Pat., 791 190; *CA*, **52**, 15597 (*synth*)

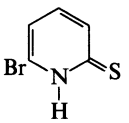
Abramovitch, R.A. *et al*, *J. Org. Chem.*, 1974, **39**, 2690 (*deriv, synth*)

Davies, J.S. *et al*, *Tetrahedron Lett.*, 1979, 5035 (*synth*)

Testaferri, L. *et al*, *Tetrahedron*, 1985, **41**, 1373 (*deriv, synth, pmr*)

6-Bromo-2(1*H*)-pyridinethione B-80256

2-Bromo-6-mercaptopyridine. 6-Bromo-2-pyridinethiol



C_5H_4BrNS M 190.063

S-*Me:* [74134-42-2]. *2-Bromo-6-(methylthio)pyridine*

C_6H_6BrNS M 204.090

Oil.

S-Me, S-*dioxide:* [98626-92-7]. *2-Bromo-6-(methylsulfonyl)pyridine, 9CI*

$C_6H_6BrNO_2S$ M 236.089

Mp 135-136°.

Furukawa, N. *et al*, *Tetrahedron Lett.*, 1983, **24**, 3243.

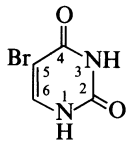
Testaferri, L. *et al*, *Tetrahedron*, 1985, **41**, 1373 (*deriv, synth, pmr*)

5-Bromo-2,4-(1*H*,3*H*)-pyrimidinedione B-80257

Updated Entry replacing B-60318

5-Bromouracil, 8CI

[51-20-7]



$C_4H_3BrN_2O_2$ M 190.984

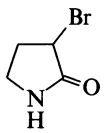
Prisms (H_2O). Mp 293°. pK_a 8.06 (H_2O), pK_a 12.7 (DMF).

▷ Mutagen. YQ9060000.

Wheeler, H.L. *et al*, *Am. Chem. J.*, 1903, **29**, 478 (*synth*)
Levene, P.A. *et al*, *Ber.*, 1912, **45**, 608 (*synth*)
Ulrich, J. *et al*, *Org. Mass Spectrom.*, 1969, **2**, 1183 (*ms*)
Ellis, P.D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 4398 (*cmr*)
Sternglanz, H. *et al*, *Biochim. Biophys. Acta*, 1975, **378**, 1 (*cryst struct*)
Yoshimura, M. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1976, **96**, 1094; *CA*, **86**, 155589g (*synth, chromatog*)
Turturo, A. *et al*, *J. Chromatogr.*, 1982, **252**, 335 (*hplc*)
Merck Index, 10th Ed., 1983, 10th Ed., no. 1414.
Srivastava, S.L. *et al*, *Spectrochim. Acta, Part A*, 1984, **40**, 675 (*uv, tautom*)
Chandrasekaran, S. *et al*, *J. Org. Chem.*, 1985, **50**, 829 (*nmr*)
Rabbani, R.S. *et al*, *J. Magn. Reson.*, 1987, **72**, 422 (*nqr*)

3-Bromo-2-pyrrolidinone B-80258

[40557-20-8]



C_4H_6BrNO M 164.001

(±)-*form* [93681-10-8]

Cryst. (Et_2O). Mp 82° (78°).

Yamada, Y. *et al*, *Agric. Biol. Chem.*, 1973, **37**, 649 (*synth, ir, pmr*)
Ikuta, H. *et al*, *J. Med. Chem.*, 1987, **30**, 1995 (*synth, pmr*)

1-Bromo-1,1,2,2-tetrafluoroethane, 9CI, 8CI B-80259

[354-07-4]

$F_2CBrCHF_2$

C_2HBrF_4 M 180.927

Shows anaesthetic props. $Bp_{625.6}$ −3.5° to −3.0°, Bp 12.5°.

[30283-90-0]

Park, J.D. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 2339 (*synth*)
Klaboe, P. *et al*, *J. Chem. Phys.*, 1961, **34**, 1819 (*ir, raman*)
Joshi, R.M., *J. Macromol. Sci., Chem.*, 1974, **8**, 861 (*props*)
Di Paolo, T. *et al*, *J. Pharmacol.*, 1979, **68**, 39 (*pharmacol*)

1-Bromo-1,1,2,2-tetrafluoro-2-iodoethane, 9CI B-80260

[421-70-5]

$F_2ClCBrF_2$

C_2BrF_4I M 306.824

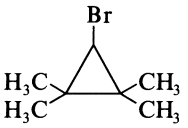
Shows anaesthetic activity. Bp 80.5-81°. n_D^{16} 1.433.

[57171-64-9]

Haszeldine, R.N., *J. Chem. Soc.*, 1953, 1764, 2075 (*synth, uv*)
Serboli, G. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 1175 (*ir*)
Cavalli, L., *J. Magn. Reson.*, 1972, **6**, 298 (*F-19 nmr*)

3-Bromo-1,1,2,2-tetramethylcyclopropane, 9CI B-80261

[3815-06-3]



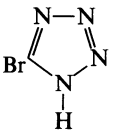
$C_7H_{13}Br$ M 177.084

Liq. Bp_{22} 51°.

Seyferth, D. *et al*, *J. Org. Chem.*, 1963, **28**, 703 (*synth, pmr*)
Hackett, M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1449 (*synth, pmr*)

5-Bromo-1*H*-tetrazole, 9CI, 8CI B-80262

[42371-37-9]



$CHBrN_4$ M 148.950

Needles (C_6H_6). Mp 156° dec. pK_a 4.13.

1-Me: [16681-79-1].

$C_2H_3BrN_4$ M 162.976

Yellow cryst. Mp 72-74°.

1-Ph: [18233-34-6].

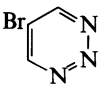
$C_7H_5BrN_4$ M 225.047

Cryst. Mp 151° dec.

Stollé, R. *et al*, *Ber.*, 1929, **62**, 1123 (*synth*)
Stollé, R. *et al*, *J. Prakt. Chem.*, 1932, **134**, 282 (*phenyl*)
Lieber, E. *et al*, *Anal. Chem.*, 1951, **23**, 1594 (*ir*)
Lieber, E. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 1792 (*props*)
Hattori, K. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 411 (*methyl*)
Ansell, J.B. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1973, 2036 (*cryst struct*)

5-Bromo-1,2,3-triazine B-80263

[114078-88-5]



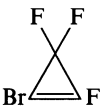
$C_3H_2BrN_3$ M 159.973

Mp 125-126° dec.

Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

1-Bromo-2,3,3-trifluorocyclopropene, 9CI B-80264

[29777-44-4]



C_3BrF_3 M 172.932

Bp 38°, Bp 44°.

McGlinchey, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1970, 1264 (*synth, F-19 nmr, ir*)
Law, D.C.F. *et al*, *J. Org. Chem.*, 1973, **38**, 771 (*synth, ir, F-19 nmr*)

2-Bromo-1,1,1-trifluoroethane, 9CI B-80265

2,2,2-Trifluoroethyl bromide

[421-06-7]

F_3CCH_2Br

$C_2H_2BrF_3$ M 162.937

Anaesthetic. d_4^{20} 1.788. Mp −93.9°. Bp 26.3°. n_D^{20} 1.3331.

[30283-91-1]

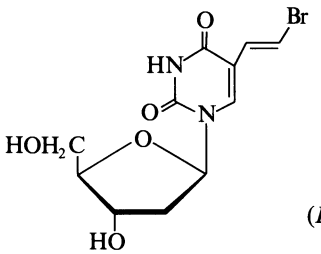
Robbins, B.H., *J. Pharmacol.*, 1946, **86**, 197 (*use*)
Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 1025 (*synth*)
Nielsen, J.R. *et al*, *J. Chem. Phys.*, 1957, **27**, 891 (*ir, raman*)
Saur, O. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 243 (*ir*)
Van der Puy, M., *J. Fluorine Chem.*, 1979, **13**, 375 (*synth*)
Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co. Ltd, 1988, 028, 029 (*F*-19 *nmr, pmr*)

5-(2-Bromovinyl)-2′-deoxyuridine B-80266

Updated Entry replacing B-20211

5-(2-Bromoethenyl)-2′-deoxyuridine, 9CI. 2′-Deoxy-5-(2-bromovinyl)uridine. ***Brivudine,*** **INN.** *Bromovinyl deoxyuridine. BVDU*

[82768-44-3]



(*E*)-*form*

$C_{11}H_{13}BrN_2O_5$ M 333.138

Antiviral agent highly active against herpes simplex.

(E)-form [69304-47-8]

Mp 123-125° dec. (141°). λ_{max} 253 (ϵ 13 100) and 295 nm(ϵ 10 300).

▷ YU7355000.

3′,5′-Di-Ac:

$C_{15}H_{17}BrN_2O_7$ M 417.212

Antiviral active against HSV-1. Needles (2-propanol). Mp 156°.

3-Me:

$C_{12}H_{15}BrN_2O_5$ M 347.165

Cryst. (H_2O).

3′-Me ether:

$C_{12}H_{15}BrN_2O_5$ M 347.165

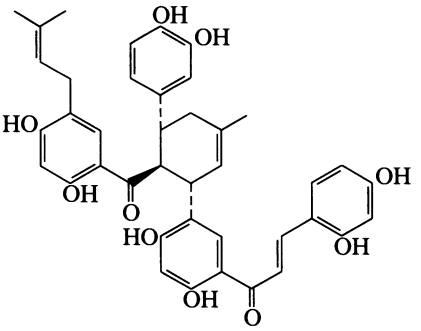
Solid.

(Z)-form [77530-02-0]

Hemihydrate. λ_{max} 234 (ϵ 11 904) and 295 nm (8 040).

Barr, P.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1981, 1665 (*synth*)
Jones, A.S. *et al*, *J. Med. Chem.*, 1981, **24**, 759 (*synth*)
Sim, T.S. *et al*, *CA*, 1982, **97**, 207422n (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 12455.
Goodchild, J. *et al*, *J. Med. Chem.*, 1983, **26**, 1252 (*synth, Z* and *E*-forms)
Robins, M.J. *et al*, *J. Org. Chem.*, 1983, **48**, 1854 (*synth*)
De Clercq, E. *et al*, *J. Antimicrob. Chemother.*, 1984, **14**, 85 (*rev, pharmacol*)
De Clercq, E. *et al*, *Pharmacol. Ther.*, 1984, **26**, 1 (*rev, synth, pharmacol*)
Parkanyi, L. *et al*, *Nucleic Acids Res.*, 1987, **15**, 4111 (*cryst struct, conformn*)
Reefschlaeger, J. *et al*, *Pharmazie*, 1987, **42**, 407 (*rev*)
Ashwell, M. *et al*, *Tetrahedron*, 1987, **43**, 4601 (*synth, props, uv, pmr*)

Brosimone B B-80267

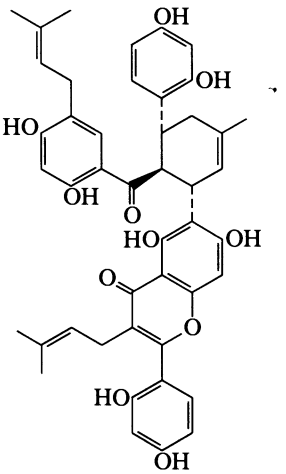


$C_{40}H_{38}O_{10}$ M 678.734

Constit. of *Brosimopsis oblongifolia*. Amorph. powder. $[\alpha]_D$ −447° (c, 0.1 in MeOH).

Messana, I. *et al*, *Heterocycles*, 1989, **29**, 683.

Brosimone D B-80268



$C_{45}H_{44}O_{11}$ M 760.836

Constit. of *Brosimopsis oblongifolia*. Amorph. powder. $[\alpha]_D$ −204° (c, 0.3 in MeOH).

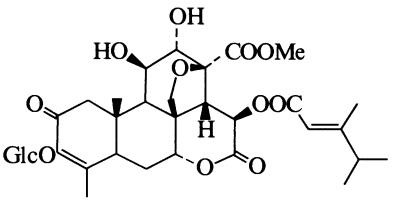
Messana, I. *et al*, *Heterocycles*, 1989, **29**, 683.

Bruceantinoside B B-80269

Updated Entry replacing B-10322

Yadanzioside P

[79439-84-2]

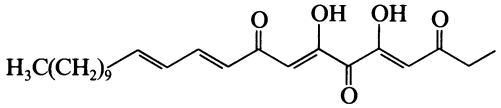


$C_{34}H_{46}O_{16}$ M 710.728

Constit. of *Brucea antidysenterica*. Amorph. powder. Mp 193-198°. $[\alpha]_D^{23}$ +7.0° (c, 0.57 in EtOH).

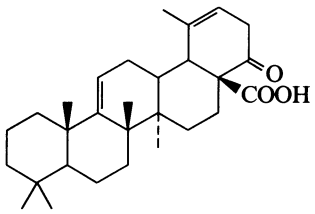
Okano, M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1981, **44**, 470 (*isol*)
Okano, M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 398 (*isol, pmr, cmr*)

Bryophollenone B-80270



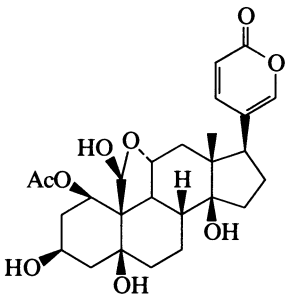
$C_{23}H_{34}O_5$ M 390.519
Constit. of *Bryophyllum pinnatum*.
Siddiqui, S. *et al*, *Phytochemistry*, 1989, **28**, 2433 (*isol, pmr, ms*)

Bryophollone B-80271



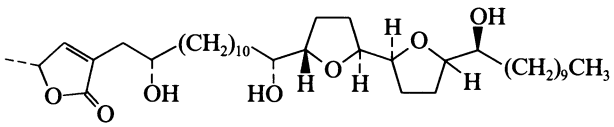
$C_{29}H_{42}O_3$ M 438.649
Constit. of *Bryophyllum pinnatum*. Cryst. (MeOH/C_6H_6). Mp 210°.
Siddiqui, S. *et al*, *Phytochemistry*, 1989, **28**, 2433 (*isol, pmr*)

Bryophyllin B B-80272



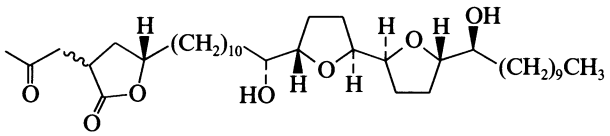
$C_{26}H_{34}O_9$ M 490.549
Constit. of *Bryophyllum pinnatum*. Amorph. powder. Mp 178-180°. $[\alpha]_D^{20}$ +20° (c, 0.1 in $CHCl_3$).
Yamagishi, T. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1071 (*isol, pmr, cmr*)

Bullatacin B-80273



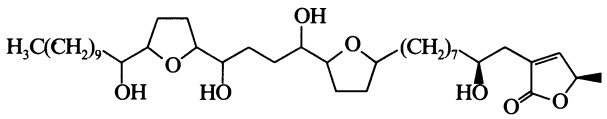
$C_{37}H_{66}O_7$ M 622.924
Constit. of *Annona bullata*. Cytotoxic agent. Cryst. (EtOAc). Mp 69-70°. $[\alpha]_D^{23}$ +13° (c, 0.004 in $CHCl_3$).
Hui, Y.-H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 463 (*isol, pmr, cmr*)

Bullatacinone B-80274



$C_{37}H_{66}O_7$ M 622.924
Constit. of *Annona bullata*. Cytotoxic agent. Cryst. (MeOH). Mp 90.5-90.7°. $[\alpha]_D^{23}$ +12.0° (c, 0.4 in $CHCl_3$).
Hui, Y.-H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 463 (*isol, pmr, cmr*)

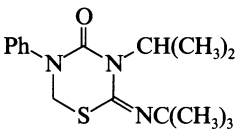
Bullatalicin B-80275



$C_{37}H_{66}O_8$ M 638.924
Constit. of *Annona bullata*. Amorph. solid. Mp 120-121°. $[\alpha]_D$ +13.25° (c, 4.0 in EtOH).
▷ Cytotoxic.
Hui, Y. *et al*, *Tetrahedron*, 1989, **45**, 6941.

Buprofezin B-80276

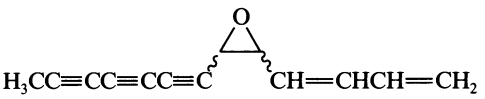
*2-[(1,1-Dimethylethyl)imino]tetrahydro-3-(1-methylethyl)-5-phenyl-4*H*-1,3,5-thiadiazin-4-one, 9CI. 2-*tert*-Butylimino-3-isopropyl-5-phenyl-1,3,5-thiadiazinan-4-one. Applaud*
[69327-76-0]



$C_{16}H_{23}N_3OS$ M 305.443
Insecticide, acaricide. Cryst. Mp 104.5-105.5°.
▷ LD_{50} 2,000 mg/Kg (rat).
Ger. Pat., 2 824 126, (1978); *ca*, **90**, 121669s (*synth*)
Kanno, H. *et al*, *Proc. Brit. Crop Prot. Comb. Pests Dis.*, 1981, **1**, 59 (*use*)
Pesticide Manual, 8th Ed., 1987, 1480.

2-(1,3-Butadienyl)-3-(1,3,5-heptatriynyl) oxirane B-80277

5,6-Epoxy-1,3-tridecadiene-7,9,11-triyne. ***Cotaepoxide***



$C_{13}H_{10}O$ M 182.221
Isol. from roots of *Anthemis cota*. Cryst. (pet. ether). Mp 66°. $[\alpha]_{546}^{20}$ −302° (c, 0.4 in Et_2O).
Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 1320; 1963, **96**, 1485 (*isol, uv, ir, struct*)

2-Buten-1-amine, 9CI B-80278

Updated Entry replacing A-01176
1-Amino-2-butene. Crotylamine
[21035-54-1]

$H_3CCH{=}CHCH_2NH_2$

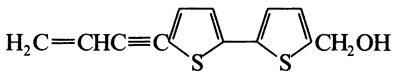
C_4H_9N M 71.122
▷ EN0702500.

(*E*)-*form* [56930-04-2]
Bp 83.6-84.2°. n_D^{25} 1.4320.
Picrate: Mp 158.3-159°.
(*Z*)-*form* [58887-05-1]
d^{29} 0.793. Bp 85-87°. n_D^{28} 1.4295.
B,HCl: Flat prisms (EtOH/Et_2O). Mp 138°.
Picrate: [55987-11-6].
Cryst. (EtOH aq.). Mp 131.5-132.5°.

Bookman, S., *Ber.*, 1895, **28**, 3114 (*synth*)
Galand, E. *et al*, *Bull. Soc. Chim. Belg.*, 1930, **39**, 529 (*synth*)
Roberts, J.D. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 2509 (*synth*)
Kjaer, A. *et al*, *Acta Chem. Scand.*, 1954, **8**, 1335 (*synth*)
Ettlinger, M.G. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 1831 (*synth*)

5-(3-Buten-1-ynyl)-5′ hydroxymethyl-2,2′-bithienyl B-80279

5′-(3-Buten-1-ynyl)-[2,2′-bithienyl]-2-methanol
[1211-41-2]



$C_{13}H_{10}OS_2$ M 246.353
Isol. from *Echinops sphaerocephalus*, *Buphthalmum salicifolium*, *B. grandiflorum* and *Bidens dahlioides*. Yellowish cryst. (CCl_4 or Et_2O/pet. ether). Mp 98°.

Ac: [1152-21-2]. ***5-Acetoxymethyl-5′-(3-buten-1-ynyl)-2,2′-bithienyl***
$C_{15}H_{12}O_2S_2$ M 288.391
Isol. from roots of *Flaveria repanda*, *E. sphaerocephalus*, *Buphthalmum salicifolium*, *B. grandiflorum* and *Bidens dahlioides*. Yellowish cryst. (pet. ether). Mp 53.5°.

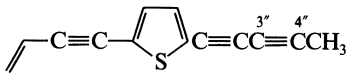
Deoxy: [1137-83-3]. ***5-(3-Buten-1-ynyl)-5′-methyl-2,2′-bithienyl***
$C_{13}H_{10}S_2$ M 230.354
Isol. from *Buphthalmum salicifolium* and *B. grandiflorum*. Light-yellow cryst. (pet. ether). Mp 61° (53-54°).

[1152-21-2]

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 1229; 1965, **98**, 155, 883, 1228; 1966, **99**, 984 (*isol, uv, ir, pmr, biosynth*)
Atkinson, R.E. *et al*, *J. Chem. Soc. C*, 1967, 2011 (*synth*)
Curtis, R.F. *et al*, *Tetrahedron*, 1967, **23**, 4419 (*uv, ir*)

2-(3-Buten-1-ynyl)-5-(1,3-pentadiynyl) thiophene B-80280

[1205-94-3]

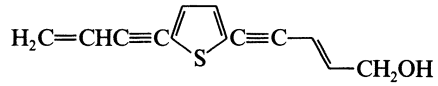


$C_{13}H_8S$ M 196.272
Isol. from roots of *Echinops sphaerocephalus*, from *Calocephalus citreus*, *Eriophyllum caespitosum*, *Ambrosia trifida* and *A. trifoliata*. Oil. Mp 5-10°. $Bp_{0.001}$ 110°.

3″,4″-Dihydro (E-): [16714-43-5]. ***2-(3-Buten-1-ynyl)-5-(3-penten-1-ynyl)thiophene***
$C_{13}H_{10}S$ M 198.288
Isol. from *Lasthenia glaberrima*, *Baeria* spp., *Bidens* spp., and *Centaurea* spp. Liq. $Bp_{0.001}$ 80°. λ_{max} 333.5, 355 nm.

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 2125; 1965, **98**, 155, 1228, 3081; 1966, **99**, 984 (*isol, uv, ir, pmr, struct*)
Sörensen, J.S. *et al*, *Acta Chem. Scand.*, 1965, **18**, 2182 (*isol, uv, ir, pmr, struct*)
Atkinson, R.E. *et al*, *Tetrahedron Lett.*, 1965, 297 (*isol, deriv*)

5-[5-(3-Buten-1-ynyl)-2-thienyl]-2-penten-4-yn-1-ol B-80281



$C_{13}H_{10}OS$ M 214.287
(*E*)-*form* [14744-66-2]
Minor constit. of roots of *Baeria* spp. Yellow cryst. (pet. ether). Mp 39°. λ_{max} 335 mm (Et_2O).

Ac: [14744-67-3]. *2-(1-Acetoxy-3-penten-1-ynyl)-5-(3-buten-1-ynyl)thiophene. 1-Acetoxy-5-[5-(3-buten-1-ynyl)-2-thienyl]-2-penten-4-yne*
$C_{15}H_{12}O_2S$ M 256.325
Cryst. (pet. ether). Mp 43.5-44°. λ_{max} 335 mm (Et_2O).

1-Aldehyde: 5-[5-(3-Buten-1-ynyl)-2-thienyl]-2-penten-4-ynal, 9CI
$C_{13}H_8OS$ M 212.272
Isol. from roots of *B.* spp. and *Veronia cotoneaster*. Cryst. (pet. ether). Mp 60°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 2125; 1967, **100**, 1200 (*isol, uv, ir, pmr, struct, synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1982, **21**, 695 (*isol, deriv*)

1-*tert*-Butoxy-1-hexyne B-80282

[113279-42-8]

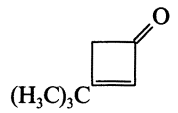
$$H_3C(CH_2)_3C{\equiv}COC(CH_3)_3$$

$C_{10}H_{18}O$ M 154.252
Oil.

Pericàs, M.A. *et al*, *Tetrahedron*, 1987, **43**, 2311 (*synth, ir, pmr, cmr, ms*)

3-*tert*-Butyl-2-cyclobuten-1-one B-80283

3-(1,1-Dimethylethyl)-2-cyclobuten-1-one, 9CI
[95904-85-1]

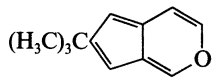


$C_8H_{12}O$ M 124.182

Schmit, C. *et al*, *Tetrahedron Lett.*, 1984, **25**, 5043 (*synth*)
Danheiser, R.L. *et al*, *Tetrahedron Lett.*, 1987, **28**, 3299 (*synth*)

6-*tert*-Butylcyclopenta[*c*]pyran B-80284

6-(1,1-Dimethylethyl)cyclopenta[c]*pyran*
[115162-91-9]



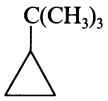
$C_{12}H_{14}O$ M 174.242
Stabilised homologue of Cyclopenta[*c*]pyran, C-80192. Lemon-yellow cryst. Mp 62° subl. Stable for several months at 4°.

Kämpchen, T. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 855 (*synth, ir, uv, pmr, cmr*)

tert-Butylcyclopropane B-80285

(1,1-Dimethylethyl)cyclopropane, 9CI

[4741-87-1]



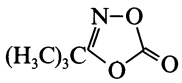
C_7H_{14} M 98.188

Kropp, P.J. *et al*, *Tetrahedron*, 1981, **37**, 3229 (*synth*)
Engel, P.S. *et al*, *J. Org. Chem.*, 1988, **53**, 4748 (*synth, ms*)

3-*tert*-Butyl-1,4,2-dioxazol-5-one B-80286

3-(1,1-Dimethylethyl)-1,4,2-dioxazol-5-one, 9CI

[114379-11-2]



$C_6H_9NO_3$ M 143.142
Liq. $Bp_{3.75}$ 70°.

Mitra, S. *et al*, *J. Org. Chem.*, 1988, **53**, 2674 (*synth, pmr, ir*)

tert-Butyl hypoiodite B-80287

[917-97-5]

$(H_3C)_3COI$

C_4H_9IO M 200.019

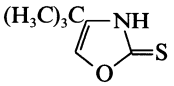
The reagent known by this name is oligomeric and two different compositions are obt. depending on the synthetic route. Homolytic and heterolytic source of iodine. Made and used in soln. V. moisture-sensitive.

Glover, S.A. *et al*, *Tetrahedron Lett.*, 1980, **21**, 2005 (*synth, use*)
Tanner, D.D. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5261 (*synth, struct, use, bibl*)
Heasley, V.L. *et al*, *J. Org. Chem.*, 1988, **53**, 198 (*props, bibl*)

4-*tert*-Butyl-2(3*H*)-oxazolethione B-80288

*4-(1,1-Dimethylethyl)-2(3*H*)-oxazolethione, 9CI*

[112683-63-3]

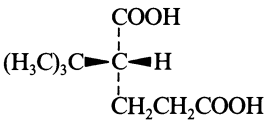


$C_7H_{11}NOS$ M 157.236
Cryst. Mp 145-147°.

Mohanraj, S. *et al*, *J. Org. Chem.*, 1988, **53**, 1113 (*synth, ir, pmr, cmr, cryst struct*)

2-*tert*-Butylpentanedioic acid B-80289

*2-(1,1-Dimethylethyl)pentanedioic acid. 2-*tert*-Butylglutaric acid*



(R)-form

$C_9H_{16}O_4$ M 188.223

(*R*)-*form* [118060-95-0]
Cryst. (toluene/hexane). Mp 94-95°. $[\alpha]_D^{20}$ +14° (c, 2 in Me_2CO).

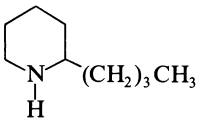
Anhydride: [118060-96-1].
$C_9H_{14}O_3$ M 170.208
Cryst. (toluene/hexane). Mp 51-52°.

Imide: [118060-97-2]. *3-*tert*-Butyl-2,6-piperidinedione. 2-*tert*-Butylglutarimide*
$C_9H_{15}NO_2$ M 169.223
Cryst. (toluene/hexane). Mp 158-159°. $[\alpha]_D^{20}$ −24° (c, 1 in MeOH).

Poloński, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 639 (*synth, cd, pmr, ir*)

2-Butylpiperidine B-80290

[72939-22-1]



$C_9H_{19}N$ M 141.256

N-*Me:* ***2-Butyl-1-methylpiperidine.*** *1-Methyl-2-butylpiperidine*
$C_{10}H_{21}N$ M 155.283
Trace alkaloid from oil of *Pimpinella acuminata* (Umbelliferae). Opt. activity not reported.

(+)-*form*
$[\alpha]_D$ +15.7°.

B,H₂PtCl₆: Mp 131-132°.

(−)-*form*
$[\alpha]_D$ −18.7°.

Tartrate salt: Needles. Mp 41-42°. Forms a dihydrate.

(±)-*form* [68144-45-6]
Liq. Bp 191-193°, Bp_{14} 75°.

B,HCl: Mp 191-193° (181-182°).

B,HBr: Mp 196-197°.

N-*Me:* Liq. Bp_{15} 75-80°.

N-*Me, picrate:* Mp 88°.

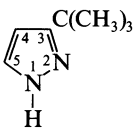
[68474-12-4]

Loffler, K. *et al*, *Ber.*, 1907, **40**, 1310 (*synth, resoln*)
Diels, O. *et al*, *Justus Liebigs Ann. Chem.*, 1937, **530**, 68 (*synth*)
Astier, A. *et al*, *Tetrahedron Lett.*, 1978, 2051 (*synth*)
Ashraf, M. *et al*, *Pak. J. Sci. Ind. Res.*, 1979, **22**, 79 (*isol, deriv*)
Scully, F.E. *et al*, *J. Org. Chem.*, 1980, **45**, 1515 (*synth, pmr, ir*)
Pirkle, W.H. *et al*, *J. Org. Chem.*, 1984, **49**, 2504 (*resoln*)

3(5)-*tert*-Butylpyrazole B-80291

3(5)-(1,1-Dimethylethyl)pyrazole

[15802-80-9]



$C_7H_{12}N_2$ M 124.185
Mp 53-54°. $Bp_{0.15}$ 127° ($Bp_{0.3}$ 76-80°) .

Elguero, J. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 3744; 1968, 707 (*synth, uv*)
Magee, W.L. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 633 (*synth*)
Cabildo, P. *et al*, *Org. Magn. Reson.*, 1984, **22**, 603 (*cmr*)
Trofimenko, S. *et al*, *Inorg. Chem.*, 1987, **26**, 1507 (*synth, pmr*)
Sorrell, T.N. *et al*, *Inorg. Chem.*, 1987, **26**, 1755 (*synth, pmr*)

4-*tert*-Butylpyrazole B-80292

4-(1,1-Dimethylethyl)pyrazole, 9CI

[105285-21-0]

$C_7H_{12}N_2$ M 124.185

Yellowish oil.

Picrate: Mp 100-102°.

Cativiela, C. *et al*, *Gazz. Chim. Ital.*, 1986, **116**, 119 (*synth, ir, uv, pmr, deriv*)

tert-Butylsulfinic acid B-80293

2-Methyl-2-propanesulfinic acid

[29099-08-9]

$(H_3C)_3CSO_2H$

$C_4H_{10}O_2S$ M 122.188

Acid not isol.

2,4-Dinitrophenyl ester: [112881-95-5].
Cryst. Mp 83-85°.

4-Nitrobenzyl ester: Cryst. (C_6H_6/pet. ether). Mp 178°.

Chloride: [31562-43-3].
C_4H_9ClOS M 140.633
Pale yellowish oil. Bp_{11} 54-57°.

Kader, A.T. *et al*, *J. Chem. Soc.*, 1962, 3425 (*synth*)
Nooi, J.R. *et al*, *Tetrahedron Lett.*, 1970, 2531 (*synth, pmr*)
Block, E. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 3921 (*deriv, synth*)
Netscher, T. *et al*, *Synthesis*, 1987, 683 (*deriv, synth, ir, pmr*)

3-Butyn-1-amine, 9CI B-80294

4-Amino-1-butyne

[14044-63-4]

$HC{\equiv}CCH_2CH_2NH_2$

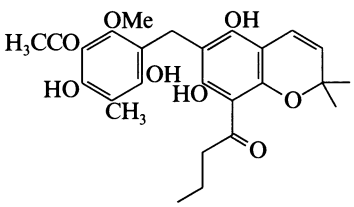
C_4H_7N M 69.106

Liq. Bp 94-95° (99°) .

Dumont, J.L. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 588 (*synth, ir*)
Taylor, E.C. *et al*, *Tetrahedron*, 1987, **43**, 5145 (*synth, ir, pmr*)

Butyrylmallotochromene B-80295

[116979-51-2]



$C_{26}H_{30}O_8$ M 470.518

See also Isobutyrylmallotochromene, I-80050. Constit. of *Mallotus japonicus*. Cytotoxic agent. Yellow needles (MeOH). Mp 175-176°.

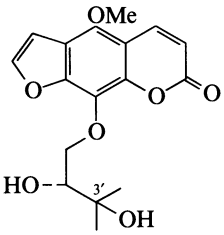
Fujita, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 708.

Byakangelicin B-80296

Updated Entry replacing B-03861

*9-(2,3-Dihydroxy-2-methylbutoxy)-4-methoxy-7*H*-furo[3,2-g][1]benzopyran-7-one, 9CI*

[19573-01-4]



Absolute configuration

$C_{17}H_{18}O_7$ M 334.325

(R)-form [482-25-7]
Constit. of Japanese drug byakusi obt. from *Angelica* spp. Mp 117-118°. Opt. rotn. data inaccessible but is thought to be dextrorotatory.

▷ LV1049000.

O-*Angeloyl:*
$C_{22}H_{24}O_8$ M 416.427
Isol. from *Seseli libanotis*. No opt. rotn. or config.

3'-Deoxy, 3'-chloro:
$C_{17}H_{17}ClO_6$ M 352.770
Isol. from *Heracleum pyrenaicum*. Mp 156-158°. $[\alpha]_D$ −28.3° ($CHCl_3$).

3'-Deoxy, 3',4'-didehydro: [35214-82-5]. ***Neobyakangelicol***
$C_{17}H_{16}O_6$ M 316.310
Isol. from roots of *A. dahurica*. Mp 106-107°. $[\alpha]_D^{20}$ −2.0° (EtOH). Abs. config. of side-chain not known.

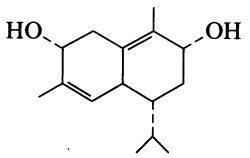
3'-Deoxy, 2'-ketone: [35214-81-4]. ***Anhydrobyakangelicin.*** *Isobyakangelicol*
$C_{17}H_{16}O_6$ M 316.310
Isol. from roots of *A. dahurica*. Mp 108-109°.

Perel'son, M.E. *et al*, *Khim. Prir. Soedin.*, 1971, 576; *CA*, **76**, 45335y (*pmr*)
Saiki, Y. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1971, **91**, 1313 (*Neobyakangelicol, Anhydrobyakangelicin*)
Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985, no. 580 (*occur*)
Fukushima, S. *et al*, *Chem. Pharm. Bull.*, 1974, **22**, 1227 (*ms*)
Kovalev, I.P. *et al*, *Farm. Zh.* (*Kiev*), 1975, **30**, 44; *CA*, **84**, 104899a (*abs config*)
González, A.G. *et al*, *An. Quim.*, 1976, **72**, 584 (*deriv*)

C

1(10),4-Cadinadiene-3,9-diol C-80001

3,9-Dihydroxy-δ-cadinene



$C_{15}H_{24}O_2$ M 236.353
Constit. of *Helichrysum dasyanthum*. Gum.

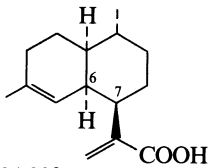
Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

4,11(13)-Cadinadien-12-oic acid C-80002

Updated Entry replacing C-70004

1,2,3,4,4a,5,6,8a-Octahydro-4,7-dimethyl-α-methylene-1-naphthaleneacetic acid,9CI. Artemisininic acid. Artemisic acid. Qing Hau acid. Arteannuic acid. Artemisinic acid

[80286-58-4]

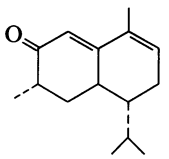


$C_{15}H_{22}O_2$ M 234.338
Isol. from *Artemisia annua*. Shows antibacterial activity. Cubes (pet. ether). Mp 131°. $[\alpha]_D$ +36° (c, 0.01 in $CHCl_3$).

6,7-Didehydro: 4,6,11(13)-Cadinatrien-12-oic acid. 6,7-Dehydroartemisinic acid
$C_{15}H_{20}O_2$ M 232.322
Constit. of *A. annua*. Cryst. (Et_2O/hexane). Mp 129-130°. $[\alpha]_D$ +317° (c,0.05 in MeOH).

Tu, Y.Y. *et al*, *Planta Med.*, 1982, **44**, 143 (*isol*)
Zhou, W. *et al*, *CA*, 1985, **103**, 160709 (*config*)
El-Feraly, F.S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 196 (*isol, deriv, pmr, cmr*)

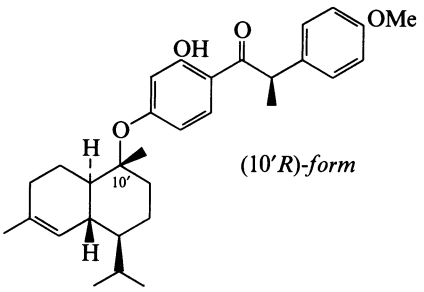
1,9-Cadinadien-3-one C-80003



$C_{15}H_{22}O$ M 218.338
Constit. of *Helichrysum petiolare*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

4-*O*-Cadinylangolensin C-80004



(10′*R*)-*form*

$C_{31}H_{40}O_4$ M 476.655

(10′R)-form [75917-91-8]
4-O-α-*Cadinylangolensin*
Isol. from *Pterocarpus angolensis* heartwood. Needles (EtOH). Mp 136°.

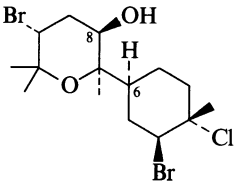
(10′S)-form [75872-84-3]
4-O-τ-*Cadinylangolensin*
Isol. from *P. angolensis* heartwood. Noncryst. Mp 44-46°.

Bezuidenhoudt, B.C.B. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 2179 (*isol, cryst struct, ms, cd, pmr, cmr*)

Caespitol C-80005

Updated Entry replacing C-00036

[50656-64-9]



$C_{15}H_{25}Br_2ClO_2$ M 432.622
Constit. of *Laurencia caespitosa*. Cryst. (hexane). Mp 109-111°.

8-Deoxy: ***Caespitane***
$C_{15}H_{25}Br_2ClO$ M 416.623
Constit. of *L. caespitosa*. Cryst. Mp 82-84°. $[\alpha]_D$ +39.8° (c, 0.89 in $CHCl_3$).

6α-Hydroxy: ***6-Hydroxycaespitol***
$C_{15}H_{25}Br_2ClO_3$ M 448.621
Constit. of *L. caespitosa*. Cryst. Mp 152-153°. $[\alpha]_D$ +11.7° (c, 0.29 in $CHCl_3$).

Gonzales, A.G. *et al*, *Tetrahedron Lett.*, 1974, 1249 (*struct*)
Gonzales, A.G. *et al*, *Tetrahedron Lett.*, 1976, 3051 (*biosynth*)
Gonzales, A.G. *et al*, *Tetrahedron Lett.*, 1979, 2719 (*cmr*)
Chang, M. *et al*, *Phytochemistry*, 1989, **28**, 1417 (*isol, cryst struct, abs config*)

4-*O*-Caffeoylshikimic acid C-80006

Isodactylifric acid

$C_{16}H_{16}O_8$ M 336.298
Isol. from unripe dates (*Phoenix dactylifera*). Tentative struct.

Maier, V.P. *et al*, *Biochem. Biophys. Res. Commun.*, 1964, **14**, 124.

5-*O*-Caffeoylshikimic acid C-80007

Neodactylifric acid

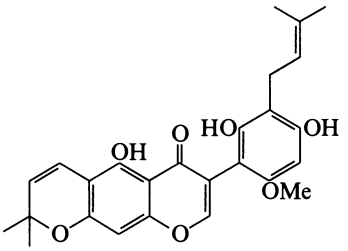
$C_{16}H_{16}O_8$ M 336.298

Isol. from unripe dates (*Phoenix dactylifera*). Tentative struct.

Maier, V.P. *et al*, *Biochem. Biophys. Res. Commun.*, 1964, **14**, 124.

Cajaisoflavone C-80008

[72578-99-5]



$C_{26}H_{26}O_7$ M 450.487

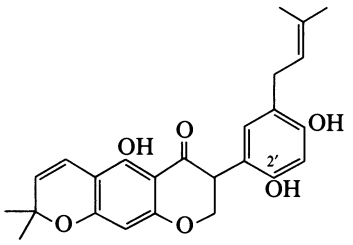
Isol. from root bark of *Cajanus cajan*. Orange semisolid.

Bhanumati, S. *et al*, *Phytochemistry*, 1979, **18**, 1254 (*isol, pmr, ms*)

Cajanone C-80009

Updated Entry replacing C-00048

[63006-48-4]



$C_{25}H_{26}O_6$ M 422.477

Constit. of *Cajanus cajan*. Shows antifungal activity.

2′-Me ether: [71765-79-2]. ***2′-O-Methylcajanone***

$C_{26}H_{28}O_6$ M 436.504

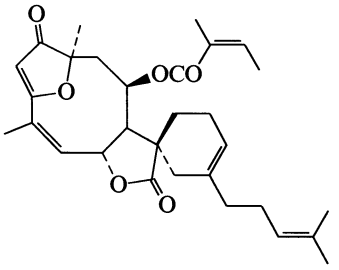
Isol. from root bark of *C. cajan*. Yellow cryst. solid (EtOAc/pet. ether). Mp 85°. Opt. inactive.

Preston, N.W., *Phytochemistry*, 1977, **16**, 143 (*isol, uv, pmr, struct*)
Bhanumati, S. *et al*, *Phytochemistry*, 1979, **18**, 693 (*deriv*)

Caleamyrcenolide C-80010

Updated Entry replacing C-20013

[84749-85-9]

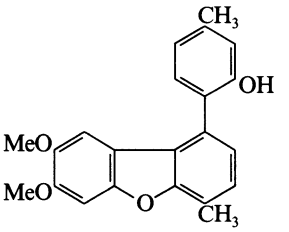


$C_{30}H_{38}O_6$ M 494.627

Constit. of *Calea hymenolepis*. Gum.

Bohlmann, F. *et al*, *Phytochemistry*, 1982, **21**, 2045.

Caleprunifolin C-80011



$C_{22}H_{20}O_4$ M 348.398

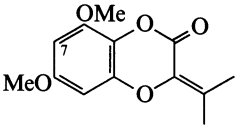
Constit. of *Calea prunifolia*. Gum.

Castro, V. *et al*, *Phytochemistry*, 1989, **28**, 2415 (*isol, pmr*)

Caleteucrin C-80012

Caleurticin

[80453-42-5]



$C_{13}H_{14}O_5$ M 250.251

Constit. of *Calea urticifolia*. Oil.

7-Methoxy: ***7-Methoxycaleteucrin***

$C_{14}H_{16}O_6$ M 280.277

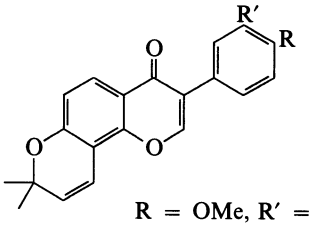
Constit. of *Calea prunifolia*. Oil.

Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 119 (*isol, pmr*)
Castro, V. *et al*, *Phytochemistry*, 1989, **28**, 2415 (*isol, pmr*)

Calopogoniumisoflavone A C-80013

*3-(4-Methoxyphenyl)-8,8-dimethyl-4*H,*8*H*-benzo[1,2-*b*:3,4-*b′*]dipyran-4-one, 9CI*

[31273-64-0]



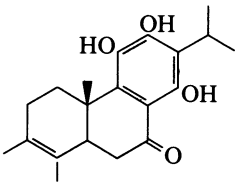
R = OMe, R′ = H

$C_{21}H_{18}O_4$ M 334.371

Isol. from seeds of *Calopogonium mucunoides*.

Vilain, C. *et al*, *Bull. Soc. R. Sci. Liege*, 1975, **44**, 306; *CA*, **84**, 74136e.

Candesalvone A C-80014



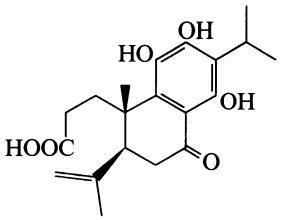
$C_{20}H_{28}O_4$ M 332.439

Constit. of *Salvia candelabrum*.

12-Me ether: Yellow plates (MeOH). Mp 209-212°.

Mendez, E. *et al*, *Phytochemistry*, 1989, **28**, 1685.

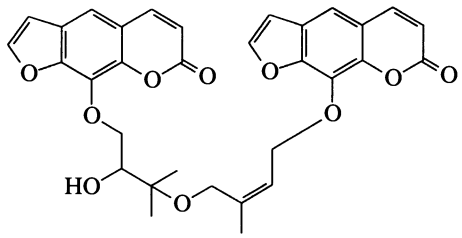
Candesalvone B C-80015



$C_{20}H_{26}O_6$ M 362.422
Constit. of *Salvia candelabrum*. Amorph. powder.
12-Me ether, Me ester: Yellow needles. Mp 85-87°.
Mendes, E. *et al*, *Phytochemistry*, 1989, **28**, 1685.

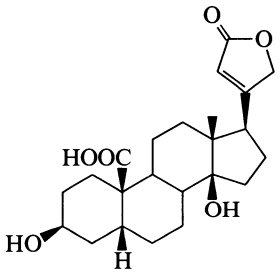
Candicanin C-80016

[36149-85-6]



$C_{32}H_{28}O_{10}$ M 572.567
MF incorr. given by the authors as $C_{32}H_{26}O_{10}$. Constit. of the roots of *Heracleum candicans*. Mp 153°.
Bandopadhyay, M. *et al*, *Tetrahedron Lett.*, 1971, 4221.

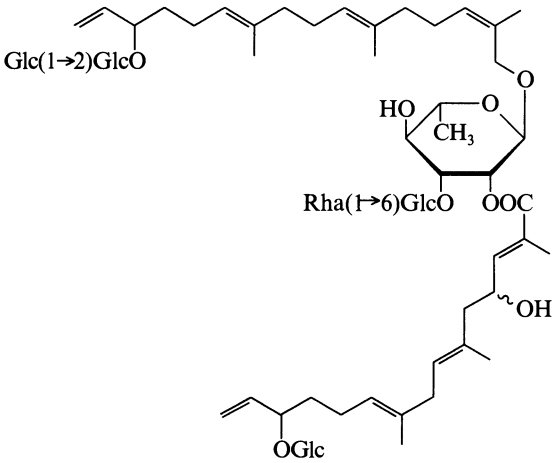
Cannogeninic acid C-80017



$C_{23}H_{32}O_6$ M 404.502
3-O-(6-Deoxy-3-O-methyl-L-glucopyranoside): ***Perusitin***
$C_{30}H_{44}O_{10}$ M 564.672
Isol. from seeds of *Thevetia peruviana*. Cryst. Mp 168-170°. $[\alpha]_D^{28.5}$ −45.5° (c, 1.37 in MeOH).
Lang, H.Y. *et al*, *CA*, 1965, **62**, 9465.

Capsianside A C-80018

[116107-40-5]



$C_{76}H_{124}O_{33}$ M 1565.796
Constit. of fruits of *Capsicum annuum*. Amorph. powder. $[\alpha]_D$ −25.1° (MeOH).
Yahara, S. *et al*, *Tetrahedron Lett.*, 1988, **29**, 1943 (*struct*)

Carbonotrithioic acid, 9CI C-80019

Updated Entry replacing C-00253
Trithiocarbonic acid
[594-08-1]

$S{=}C(SH)_2$

CH_2S_3 M 110.225
Liq. Mp −26.9°. Salts give red aq. solns.
Di-Na salt: Yellow needles (EtOH). Mp 80°.
Di-Me ester: [2314-48-9].
$C_3H_6S_3$ M 138.278
Yellow oil. Bp_{10} 90°.
Di-Et ester:
$C_5H_{10}S_3$ M 166.332
Yellow oil. Bp_7 130°.
Yeoman, E.W., *J. Chem. Soc.*, 1921, 38 (*salts*)
Gattow, G. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **321**, 143 (*synth, ir, uv*)
Philippot, E., *Rev. Chim. Miner.*, 1967, **4**, 643 (*salts, rev*)
Tomita, K. *et al*, *Chem. Pharm. Bull.*, 1972, **20**, 2302 (*deriv*)
Barbero, M. *et al*, *Synthesis*, 1988, 22 (*Di-Me ester, synth, pmr, use*)

N,N'-Carbonylbisglycine, 9CI C-80020

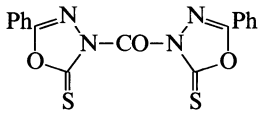
N,N'-*Bis(carboxymethyl)urea. Urea* N,N'-*diacetic acid*

$HOOCCH_2NHCONHCH_2COOH$

$C_5H_8N_2O_5$ M 176.129
Cryst. (H_2O). Mp 204-206° (188-189°).
Di-Me ester: [72129-70-5].
$C_7H_{12}N_2O_5$ M 204.182
Cryst. ($CHCl_3$/hexane). Mp 155-156°.
Di-Et ester: [7150-63-2].
$C_9H_{16}N_2O_5$ M 232.236
Cryst. ($CHCl_3$). Mp 147-148° (143-145°).
Wessely, F. *et al*, *Hoppe Seyler's Z. Physiol. Chem.*, 1928, **174**, 306 (*synth*)
Kondo, K. *et al*, *Synthesis*, 1979, 735 (*synth, ir*)
Buntain, I.G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3175 (*synth, ir, pmr*)

3,3′-Carbonylbis[5-phenyl-1,3,4-oxadiazole-2(3*H*)-thione], 9CI C-80021

[122350-19-0]



$C_{17}H_{10}N_4O_3S_2$ M 382.423

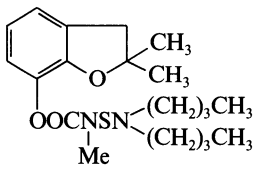
Stable one-pot condensing agent. Pale-yellow granular cryst. (C_6H_6). Mp 202°.

Saesuga, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1989, **62**, 539 (*synth, use*)

Carbosulfan C-80022

2,3-Dihydro-2,2-dimethyl-7-benzofuranyl [(di-butylamino)thio]methylcarbamate, 9CI. Marshal. Advantage

[55285-14-8]



$C_{20}H_{32}N_2O_3S$ M 380.550

Systemic insecticide for control of soil pests. Brown viscous liq.

▷ LD_{50} 200 mg/kg (Rats).

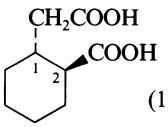
Ger. Pat., 2 433 680, (1975); *CA*, **82**, 156050 (*synth*)

Maitlen, E.C. *et al*, *Proc. Brit. Crop Prot. Comb. Pests Dis.*, 1979, **2**, 557 (*use*)

Pesticide Manual, 8th Ed., 1987, 2060.

2-Carboxycyclohexaneacetic acid, 9CI C-80023

Hexahydrohomophthalic acid



(1*R*,2*S*)-*form*

$C_9H_{14}O_4$ M 186.207

(1R,2S)-form

(+)-trans-*form*

Mp 116°. $[\alpha]_D^{20}$ +40.1° (in dioxan).

*Anhydride: Hexahydro-1*H*-2-benzopyran-*1,3(4H)-*dione, 9CI*

$C_9H_{12}O_3$ M 168.192

Cryst. (toluene/hexane). Mp 111-112°. $[\alpha]_D^{20}$ −81° ($CHCl_3$).

(1R*,2R*)-form

(+)-cis-form

Cryst. Mp 82°. $[\alpha]_D^{20}$ +12.0°.

Anhydride: Cryst. Mp 88°. $[\alpha]_D^{20}$ −30.3°.

(1RS,2RS)-form

(±)-cis-*form*

Mp 147°.

(1RS,2SR)-form

(±)-trans-*form*

Mp 161°.

[14715-37-8]

Benner, E. *et al*, *Acta Chem. Scand.*, 1954, **8**, 64 (*synth, resoln, bibl*)

Poloński, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 639 (*synth, cd*)

(2-Carboxyethyl)dimethylsulfonium(1+) C-80024

Dimethyl-β-propriothetin

[6708-36-7]

$Me_2S^{\oplus}CH_2CH_2COOH$

$C_5H_{11}O_2S^{\oplus}$ M 135.207 (ion)

Isol. from green and red algae, e.g. *Enteromorpha intestinalis, Ulva lactuca*. Also from*Spartina anglica*. Biol. precursor of dimethyl sulfide.

Chloride: [4337-33-1].

$C_5H_{11}ClO_2S$ M 170.659

Needles (EtOH). Mp 134° dec.

Challenger, F. *et al*, *J. Chem. Soc.*, 1948, 1591 (*isol*)

Greene, R.C. *et al*, *J. Biol. Chem.*, 1962, **237**, 2251 (*biosynth*)

Larher, F. *et al*, *Phytochemistry*, 1977, **16**, 2019 (*isol*)

Blunden, G. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 965 (*nmr*)

4-(2-Carboxyethyl)-4-nitroheptanedioic acid, 9CI C-80025

[59085-15-3]

$O_2NC(CH_2CH_2COOH)_3$

$C_{10}H_{15}NO_8$ M 277.230

Solid. Mp 186°.

Tri-Et ester:

$C_{16}H_{27}NO_8$ M 361.391

Mp 186°.

Trinitrile: [1466-48-4]. *Tris(2-cyanoethyl)nitromethane*

$C_{10}H_{12}N_4O_2$ M 220.230

Mp 116.0-118.0°.

▷ Synth v. exothermic.

Bruson, H.A. *et al*, *J. Am. Chem. Soc.*, 1943, **65**, 23 (*nitrile*)

Šorm, F. *et al*, *Collect. Czech. Chem. Commun.*, 1954, **19**, 298 (*synth*)

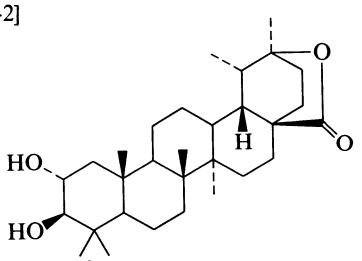
Newkome, G.R. *et al*, *J. Org. Chem.*, 1988, **53**, 5552 (*synth, nitrile, pmr, cmr*)

Careyagenolide C-80026

Updated Entry replacing C-20049

2α,3β-Dihydroxy-28,20β-taraxastanolide

[84749-88-2]



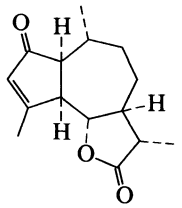
$C_{30}H_{48}O_4$ M 472.707

Constit. of *Careya arborea*. Cryst. (MeOH). Mp 299° dec.

Das, M.C. *et al*, *Phytochemistry*, 1982, **21**, 2069.

Carpesialactone C-80027

[82460-83-1]



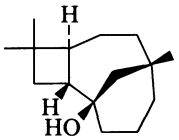
$C_{15}H_{20}O_3$ M 248.321

The identity of Bohlmann's sample having stereochem. as illus. with an earlier sample of undetd. stereochem. is not certain. Isol. from seeds of *Carpesium abrotanoides* and roots of *Hypochoeris oligocephala*. Oil or gum.

Kariyone, T. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1955, **75**, 39; *ca*, **50**, 890 (*struct*)
Naito, S., *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1955, **75**, 93, 325; *ca*, **50**, 891, 1680 (*struct, synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1982, **21**, 460 (*isol, struct*)

β-Caryophyllene alcohol C-80028

[472-97-9]



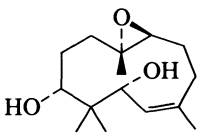
$C_{15}H_{26}O$ M 222.370

Constit. of Palmarosa and other oils. Oil.

Barrow, C.J. *et al*, *Aust. J. Chem.*, 1988, **41**, 1755 (*pmr, cmr*)

Caucalol C-80029

Updated Entry replacing C-00445



$C_{15}H_{26}O_3$ M 254.369

Di-Ac:

$C_{19}H_{30}O_5$ M 338.443

Constit. of *Caucalis scabra*. Cryst. Mp 121-122°. $[\alpha]_D^{15.5}$ +33.4° ($CHCl_3$).

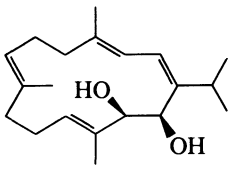
Sasaki, S. *et al*, *Tetrahedron Lett.*, 1966, 623.

1(14),4,8,12-Cembratetraene-2,3-diol C-80030

Updated Entry replacing S-50015

Sarcophytol B

[72629-68-6]



$C_{20}H_{32}O_2$ M 304.472

Constit. of *Sarcophyton glaucum* and the coral *Alcyonium flaccidum*. Cryst. (Me_2CO). Mp 125-126.5°. $[\alpha]_D$ +164° (c, 1 in $CHCl_3$).

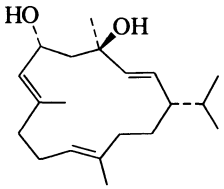
Kobayashi, M. *et al*, *Chem. Pharm. Bull.*, 1979, **27**, 2382 (*isol*)
Kashman, Y. *et al*, *J. Org. Chem.*, 1981, **46**, 3592 (*isol*)
Czarkie, D. *et al*, *Tetrahedron*, 1985, **41**, 1049 (*isol*)
McMurry, J.E. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1173 (*synth, cryst struct*)

2,7,11-Cembratriene-4,6-diol C-80031

Updated Entry replacing C-70030

4,8,13-Duvatriene-1,3-diol

[57605-80-8]



(1*S*,2*E*,4*R*,6*R*,7*E*,11*E*)-*form*

$C_{20}H_{34}O_2$ M 306.487

Cryst.

(1S,2E,4R,6R,7E,11E)-form [58190-98-0] ***β-Cembrenediol***

Constit. of tobacco. Plant growth inhibitor. Cryst. Mp 150-152° (123°). $[\alpha]_D$ +40° ($CHCl_3$).

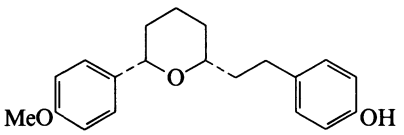
(1S,2E,4S,6R,7E,11E)-form [75282-01-8] ***α-Cembrenediol***

Constit. of tobacco. Mp 118-120°. $[\alpha]_D$ +100° ($CHCl_3$).

Springer, J.P. *et al*, *Tetrahedron Lett.*, 1975, 2737 (*isol*)
Chang, S.Y. *et al*, *Phytochemistry*, 1976, **15**, 961 (*isol*)
Wahlberg, I. *et al*, *Acta Chem. Scand.*, *Ser. B*, 1982, **36**, 443 (*isol*)
Crombie, L. *et al*, *Phytochemistry*, 1988, **27**, 1685 (*biosynth*)
Begley, M.J. *et al*, *Phytochemistry*, 1988, **27**, 1695 (*cryst struct*)
Marshall, J.A. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1055 (*synth, abs config*)

Centrolobin C-80032

*4-[2-[Tetrahydro-6-(4-methoxyphenyl)-2*H*-pyran-2-yl]ethyl]phenol, 9CI*



$C_{20}H_{24}O_3$ M 312.408

(+)-form [30358-99-7]

Isol. from wood of *Centrolobium robustum*. Cryst. Mp 87°. $[\alpha]_D^{20}$ +97° (c, 0.4 in $CHCl_3$).

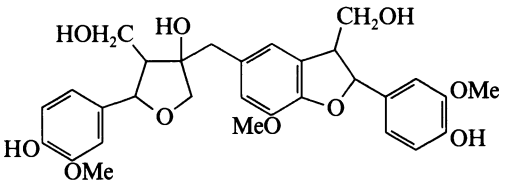
(±)-form

Oil. $Bp_{0.03}$ 190°.

de Albuquerque, I.L. *et al*, *Gazz. Chim. Ital.*, 1964, **94**, 287 (*isol, ir, pmr, struct*)
Galeffi, C. *et al*, *Gazz. Chim. Ital.*, 1965, **95**, 95 (*synth*)
Craveiro, A.A. *et al*, *Phytochemistry*, 1970, **9**, 1975 (*isol*)
Nagal, M. *et al*, *Chem. Pharm. Bull.*, 1986, **34**, 1056 (*abs config*)

Cerberalignan D C-80033

[119403-22-4]



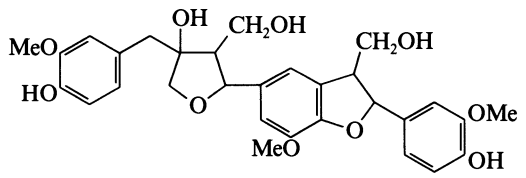
$C_{30}H_{34}O_{10}$ M 554.593

Constit. of *Cerbera manghas* and *C. odollam*. Solid. $[\alpha]_D^{25}$ −50.6° (c, 0.98 in MeOH).

Abe, F. *et al*, *Phytochemistry*, 1988, **27**, 3627.

Cerberalignan E C-80034

[119403-23-5]

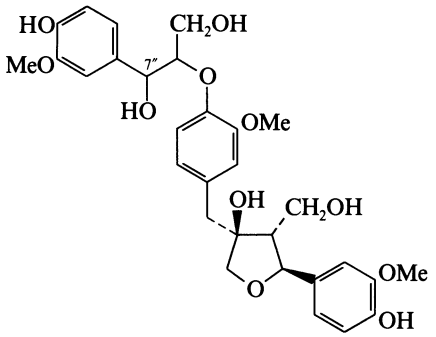


$C_{30}H_{34}O_{10}$ M 554.593
Constit. of *Cerbera manghas* and *C. odollam*. Solid. $[\alpha]_D^{24}$ −35.9° (c, 0.4 in MeOH).

Abe, F. *et al*, *Phytochemistry*, 1988, **27**, 3627.

Cerberalignan F C-80035

[119420-37-0]



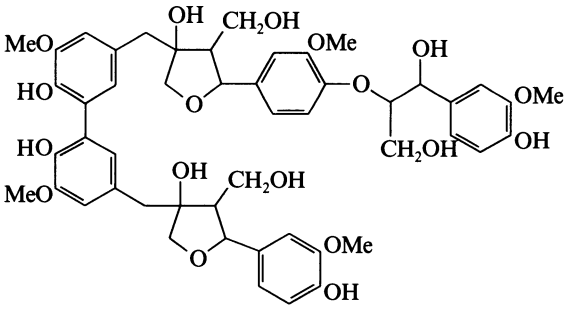
$C_{30}H_{36}O_{11}$ M 572.608
Constit. of *Cerbera manghas* and *C. odollam*. Solid. $[\alpha]_D^{28}$ −49° (c, 0.4 in MeOH).

7″-Epimer: [119478-88-5]. ***Cerberalignan G***
$C_{30}H_{36}O_{11}$ M 572.608
Constit. of *C. manghas* and *C. odollam*. Solid. $[\alpha]_D^{28}$ −68.4° (c, 0.5 in MeOH).

Abe, F. *et al*, *Phytochemistry*, 1988, **27**, 3627.

Cerberalignan H C-80036

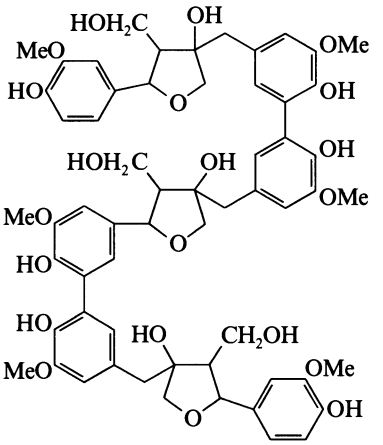
[119420-38-1]



$C_{50}H_{58}O_{18}$ M 946.997
Constit. of *Cerbera manghas* and *C. odollam*. Solid. $[\alpha]_D^{25}$ −62° (c, 0.39 in MeOH).

Abe, F. *et al*, *Phytochemistry*, 1988, **27**, 3627.

Cerberalignan I C-80037



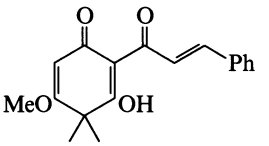
$C_{60}H_{68}O_{21}$ M 1125.185
Constit. of *Cerbera manghas* and *C. odollam*. Solid. $[\alpha]_D^{25}$ −76.7° (c, 0.72 in MeOH).

Abe, F. *et al*, *Phytochemistry*, 1988, **27**, 3627.

Ceroptene C-80038

3-Hydroxy-5-methoxy-4,4-dimethyl-2-(1-oxo-3-phenyl-2-propenyl)-2,5-cyclohexadien-1-one. 2-Cinnamoyl-3-hydroxy-5-methoxy-4,4-dimethyl-2,5-cyclohexadien-1-one

[56015-03-3]

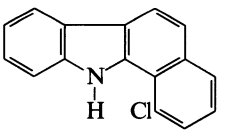


$C_{18}H_{18}O_4$ M 298.338
Mixt. of tautomers in soln. Probable struct. Isol. from the yellow leaf deposit of ferns *Pitryogramma triangularis*. Yellow prisms or plates (MeOH). Mp 137-140°.

Forsen, S. *et al*, *Acta Chem. Scand.*, 1959, **13**, 750, 1383 (*isol, ir, ms, pmr, struct*)
Dreyer, D.L. *et al*, *Tetrahedron*, 1975, **31**, 287 (*cmr*)

1-Chlorobenzo[*a*]carbazole C-80039

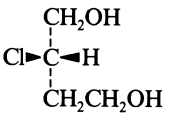
[111960-32-8]



$C_{16}H_{10}ClN$ M 251.714
Cryst. (EtOH). Mp 114-115°.

Katritzky, A.R. *et al*, *J. Org. Chem.*, 1988, **53**, 794 (*synth, pmr*)

2-Chloro-1,4-butanediol, 9CI C-80040



$C_4H_9ClO_2$ M 124.567

(S)-form [101021-55-0]
Pale yellow oil. $Bp_{0.5}$ 95-104°. $[\alpha]_D^{19}$ −45.0° (c, 1.2 in MeOH).

[101021-57-2]

Kunec, E.K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 1089 (*synth, ir, pmr*)

4-Chloro-2-buten-1-amine, 9CI C-80041

Updated Entry replacing C-50094

1-Amino-4-chloro-2-butene

$ClCH_2CH{=}CHCH_2NH_2$

C_4H_8ClN M 105.567

(E)-form

B,HCl: [100350-86-5].
Cryst. (Me_2CO). Mp 152-153° dec.

(Z)-form

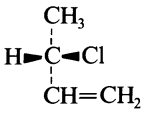
B,HCl: [7153-66-4].
Sticky cryst. prod.

Gajda, T. *et al*, *Justus Liebigs Ann. Chem.*, 1986, 992 (*synth, ir, pmr*)
Brandänge, S. *et al*, *Synthesis*, 1988, 347 (*synth, pmr, cmr*)

3-Chloro-1-butene C-80042

Updated Entry replacing C-00843

[563-52-0]



(*S*)-*form*
Absolute configuration

C_4H_7Cl M 90.552

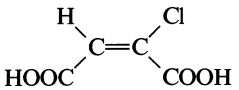
(S)-form [35729-37-4]
$[\alpha]_D^{25}$ +15.1° (neat) (25% opt. pure).

(±)-form
Bp_{766} 64°.

Kharasch, M.S. *et al*, *J. Org. Chem.*, 1938, **2**, 489 (*synth*)
Young, W.G. *et al*, *J. Org. Chem.*, 1961, **26**, 245 (*abs config*)
Normant, J.F. *et al*, *Bull. Soc. Chim. Fr.*, 1972, **7**, 2854 (*synth*)
Snyder, E.I. *et al*, *J. Org. Chem.*, 1972, **37**, 1466 (*synth*)
Magid, R.M. *et al*, *Tetrahedron Lett.*, 1977, 2999 (*synth*)

2-Chloro-2-butenedioic acid, 9CI C-80043

Updated Entry replacing C-00845



(*E*)-*form*

$C_4H_3ClO_4$ M 150.518

(E)-form [617-43-6]
Chloromaleic acid
Cryst. ($Et_2O/CHCl_3$). Insol. pet. ether. Mp 114° (sinters at 96°). Heat at 180° → anhydride.

Di-Me ester: [19393-45-4].
$C_6H_7ClO_4$ M 178.572
Bp_{18} 106.5°.
▷ ON0525000.

Anhydride: 3-Chloro-2,5-furandione
C_4HClO_3 M 132.503
Mp 33°. Bp 196°, Bp_8 78°.

(Z)-form [617-42-5]
Chlorofumaric acid
Plates (AcOH). Sol. H_2O, Et_2O. Mp 191-192°. pK_{a1} 7.76, pK_{a2} 5.81. Sublimes.
▷ LT1050000.

Di-Me ester: [5331-33-9].
Bp 224°, Bp_{15} 108°.

Di-Et ester: [10302-94-0]. *Diethyl chlorofumarate*
$C_8H_{11}ClO_4$ M 206.625
Fungicide, algicide, lubricant for nylon fibre finishing and in textile pastes. $Bp_{0.75}$ 100-105°.

Dichloride: [17096-37-6].
$C_4Cl_2O_2$ M 150.948
Bp 185-187° part. dec.

Dinitrile: 1-Chloro-1,2-dicyanoethylene
C_4HClN_2 M 112.518
Bp 172°.

[6910-76-5]

van der Riet, B., *Justus Liebigs Ann. Chem.*, 1894, **280**, 229 (*synth*)
v. Auwers, K. *et al*, *Ber.*, 1929, **62**, 1685 (*synth*)
Roedig, A. *et al*, *Justus Liebigs Ann. Chem.*, 1965, **683**, 30 (*synth*)
Maas, G. *et al*, *Justus Liebigs Ann. Chem.*, 1965, **686**, 55 (*synth*)
Mai, K. *et al*, *Chem. Ind.* (*London*), 1986, 670 (*synth, ester, use*)
Akhtar, M. *et al*, *Tetrahedron*, 1987, **43**, 5899 (*synth, ir, pmr, cmr, ms*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 839.

4-Chloro-2-butyn-1-ol C-80044

[13280-07-4]

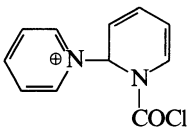
$ClCH_2C{\equiv}CCH_2OH$

C_4H_5ClO M 104.536

Dupont, G. *et al*, *Bull. Soc. Chim. Fr.*, 1954, 816.

1′-(Chlorocarbonyl)-1′,2′-dihydro-1,2′-bipyridinium (1+), 9CI C-80045

1-[2-(Chloroformyl)-2-azacyclohexa-3,5-dienyl]pyridinium



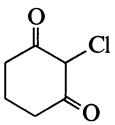
$C_{11}H_{10}ClN_2O^{\oplus}$ M 221.665 (ion)

Chloride: [117371-69-4]. *Phosgene-in-a-can*
$C_{11}H_{10}Cl_2N_2O$ M 257.118
Prod. of reaction of excess pyridine with phosgene. Useful source of phosgene. Light yellow solid. Mp 84-87° dec. Thermally stable, liberates phosgene in soln.

King, J.A. *et al*, *J. Org. Chem.*, 1988, **53**, 6145 (*synth, ir, pmr, cmr*)

2-Chloro-1,3-cyclohexanedione C-80046

[932-23-0]



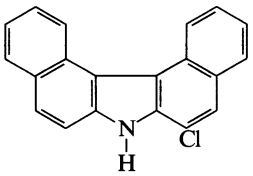
$C_6H_7ClO_2$ M 146.573

Me ether: [18369-67-0]. *2-Chloro-3-methoxy-2-cyclohexen-1-one, 9CI*
$C_7H_9ClO_2$ M 160.600
Cryst. (EtOAc). Mp 90-92°.

Shepherd, R.G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 2153 (*synth, deriv, pmr, ir*)

6-Chlorodibenzo[c,g]carbazole C-80047

[111960-36-2]



$C_{20}H_{12}ClN$ M 301.774
Cryst. (EtOH). Mp 193-195°.

Katritzky, A.R. *et al*, *J. Org. Chem.*, 1988, **53**, 794 (*synth, pmr*)

1-Chloro-1,2-difluoroethene, 9CI C-80048

[359-04-6]

FClC=CHF

C_2HClF_2 M 98.479
−15° to −12° (−6° to −4°) . Prob. mixt. of geom. isomers.

[2837-86-7, 27156-04-3, 30860-28-7]

Birchall, J.M. *et al*, *J. Chem. Soc.*, 1961, 2204 (*synth*)
Fuller, G. *et al*, *Tetrahedron*, 1962, **18**, 123 (*synth*)
Barlow, M.G., *J. Chem. Soc., Chem. Commun.*, 1966, 703 (*F nmr*)
Craig, N.C. *et al*, *J. Phys. Chem.*, 1971, **75**, 1453 (*isom*)
Syrvatka, B.G. *et al*, *Zh. Org. Khim.*, 1972, **8**, 1553 (*ms*)
Ruehl, E., *Can. J. Chem.*, 1985, **63**, 1949 (*uv*)

2-Chloro-1,1-difluoroethene, 9CI C-80049

2,2-Difluorovinyl chloride

[359-10-4]

F_2C=CHCl

C_2HClF_2 M 98.479
Gas. Mp −138.5°. Bp −19.0°.

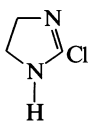
▷ Flammable.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 1025 (*synth*)
Chandra, S., *J. Phys. Chem.*, 1967, **71**, 1927 (*microwave*)
Torkelson, T.R. *et al*, *Toxicol. Appl. Pharmacol.*, 1971, **19**, 1 (*tox*)
Scott, J.D. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2634 (*uv*)
Mackenzie, M.W., *Spectrochim. Acta, Part A*, 1984, **40**, 279 (*ir*)
Osten, H.J. *et al*, *J. Chem. Phys.*, 1985, **83**, 5434 (*F-19 nmr*)

2-Chloro-4,5-dihydro-1*H*-imidazole, 9CI C-80050

2-Chloro-2-imidazoline

[54255-11-7]



$C_3H_5ClN_2$ M 104.539
Free base decomposes at r.t.

B,HCl: [54255-14-0].
Cryst. (EtOH). Mp 189-190°.

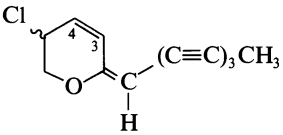
B,H_2SO_4: [54255-12-8].
Cryst. (MeOH). Mp 161-162° dec.

Trani, A. *et al*, *J. Heterocycl. Chem.*, 1974, **11**, 257 (*synth, ir, pmr*)

5-Chloro-5,6-dihydro-2-(2,4,6-octatriynylidene)-2*H*-pyran, 9CI C-80051

Updated Entry replacing C-00961

[2271-20-7]



(*E*)-*form*

$C_{13}H_9ClO$ M 216.666

(E)-form [37940-06-0]
Constit. of roots of *Anaphalis triplinervis*. Yellow cryst. (pet. ether). $[\alpha]_D^{20}$ +526° (c, 0.118 in EtOH). Dec. >80°. λ_{max} 269.5 (ϵ 25 300), 341.5 (23 900).

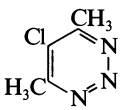
3,4-Epoxide: [6558-99-2]. *5-Chloro-2-(2,4,6-octatriynylidene)-3,7-dioxabicyclo[4.1.0]heptane, 9CI. 5-Chloro-5,6-dihydro-3,4-epoxy-2-(2,4,6-octatriynylidene)-2H-pyran*
$C_{13}H_9ClO_2$ M 232.666
Isol. from roots of *A. triplinervis*. Yellowish cryst. (pet. ether). Mp 87°.

(Z)-form
Constit. of *A. margaritacea* and *A. triplinervis*. Light-yellow cryst. or oil. Mp 73°. $[\alpha]_D^{20}$ −219° (c, 0.49 in Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1416; 1966, **99**, 1648; 1972, **105**, 3036; 1973, **106**, 1337 (*isol, uv, ir, pmr, struct, synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1978, **17**, 1917 (*isol, deriv*)

5-Chloro-4,6-dimethyl-1,2,3-triazine C-80052

[109520-02-7]



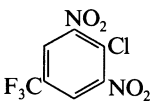
$C_5H_6ClN_3$ M 143.575
Needles (hexane). Mp 89-90°.

Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

2-Chloro-1,3-dinitro-5-(trifluoromethyl) benzene, 9CI C-80053

4-Chloro-α,α,α-trifluoro-3,5-dinitrotoluene. 3,5-Dinitro-4-chlorobenzotrifluoride

[393-75-9]



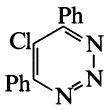
$C_7H_2ClF_3N_2O_4$ M 270.552
Cryst. Mp 58° (53-57°).

▷ Acute oral toxin, mutagenic.

Jurgens, H.R. *et al*, *J. Org. Chem.*, 1960, **25**, 1710 (*synth*)
Hill, J.R. *et al*, *Org. Magn. Reson.*, 1977, **9**, 589 (*C-13 nmr, F-19 nmr*)
Bucchi, A.R. *et al*, *Ann. Ist. Super. Sanita*, 1983, **19**, 351 (*tox*)
Schaefer, T. *et al*, *Can. J. Chem.*, 1983, **61**, 2779 (*F-19 nmr*)
Stemmler, E.A. *et al*, *Biomed. Environ. Mass Spectrom.*, 1987, **14**, 417 (*ms*)

5-Chloro-4,6-diphenyl-1,2,3-triazine C-80054

[114078-87-4]



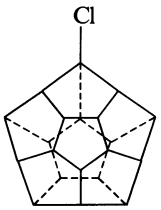
$C_{15}H_{10}ClN_3$ M 267.717
Needles (hexane/Et_2O). Mp 159-160°.

Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

Chlorododecahedrane C-80055

*1-Chlorohexadecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene, 9CI*

[112896-28-3]



$C_{20}H_{19}Cl$ M 294.823
Solid. Mp >280°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1303 (*synth, cmr*)

Chlorofluoroiodomethane C-80056

[1512-28-3]

CHClFI

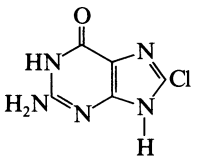
CHClFI M 194.375
Light sensitive liq. Bp 76°, Bp_{150} 35°.

Hazeldine, R.N., *J. Chem. Soc.*, 1952, 4259 (*synth*)
Samajajulu, G.R. *et al*, *J. Magn. Reson.*, 1979, **33**, 559 (*C-13 nmr*)
Kudchadker, A.P. *et al*, *J. Phys. Chem. Ref. Data*, 1979, **8**, 499 (*props*)

8-Chloroguanine, 8CI C-80057

*2-Amino-8-chloro-1,7-dihydro-6*H*-purin-6-one, 9CI. 2-Amino-8-chloro-6-hydroxypurine*

[22052-03-5]



$C_5H_4ClN_5O$ M 185.572
B,HCl: [34618-09-2].
Cryst. (2M HCl).

Wölcke, U. *et al*, *Tetrahedron Lett.*, 1969, 785 (*synth*)
Birdsall, N.J.M. *et al*, *Tetrahedron*, 1971, **27**, 5969 (*synth*)
Ryu, E.K. *et al*, *J. Org. Chem.*, 1981, **46**, 2819 (*synth*)

6-Chloro-1-hexene C-80058

[928-89-2]

$H_2C{=}CH(CH_2)_3CH_2Cl$

$C_6H_{11}Cl$ M 118.606
Liq. Bp 128-130°, Bp_{32} 55°.

Black, H.K. *et al*, *J. Chem. Soc.*, 1953, 1785 (*synth*)
Jenkins, C.L. *et al*, *J. Org. Chem.*, 1971, **36**, 3103 (*synth*)
Ashby, E.C. *et al*, *J. Org. Chem.*, 1988, **53**, 6068 (*synth, pmr, ms*)

2-Chloro-1-hexen-3-ol, 9CI, 8CI C-80059

[29279-85-4]

$H_3CCH_2CH_2CH(OH)CCl{=}CH_2$

$C_6H_{11}ClO$ M 134.605
(±)-*form*
Liq. Bp_3 47.5-49°. n_D^{20} 1.4588.

Bianchini, J.P. *et al*, *Tetrahedron*, 1970, **26**, 3401 (*synth*)

2-Chloro-4-hexen-3-ol C-80060

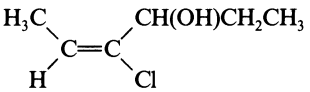
$H_3CCH{=}CHCH(OH)CHClCH_3$

$C_6H_{11}ClO$ M 134.605
Cryst. (pet. ether), Liq. Mp 109-110°. Bp_{17} 72-79°. n_D^{22} 1.4669 Mixt. of stereoisomers.

[70040-78-7, 70041-11-1, 70041-12-2, 70041-13-3]

Sauleau, J., *Bull. Soc. Chim. Fr.*, Part II, 1978, 474 (*synth, ir*)

4-Chloro-4-hexen-3-ol, 9CI, 8CI C-80061



$C_6H_{11}ClO$ M 134.605
(±)-(*E*)-*form* [96943-38-3]
Liq. $Bp_{0.1}$ 45-48°.

Barluenga, J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1985, 447 (*synth, pmr*)

6-Chloro-2-hexen-1-ol, 9CI, 8CI C-80062

$ClCH_2CH_2CH_2CH{=}CHCH_2OH$

$C_6H_{11}ClO$ M 134.605
(*Z*)-*form* [76047-81-9]
Liq. $Bp_{0.3}$ 70-72°, Bp_1 54-58°.

Holton, R.A. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 2124 (*synth, pmr, ir*)
Brennan, J.P. *et al*, *Tetrahedron*, 1986, **42**, 6719 (*synth, ir, pmr, ms*)

6-Chloro-3-hexen-1-ol, 9CI, 8CI C-80063

$ClCH_2CH_2CH{=}CHCH_2CH_2OH$

$C_6H_{11}ClO$ M 134.605
(*Z*)-*form*
Liq. $Bp_{0.5}$ 63°. n_D^{26} 1.4742.

Meinwald, J. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 4087 (*synth*)

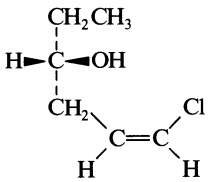
6-Chloro-4-hexen-1-ol, 9CI, 8CI C-80064

$ClCH_2CH{=}CHCH_2CH_2CH_2OH$

$C_6H_{11}ClO$ M 134.605
(*Z*)-*form* [104410-97-1]
Liq.

Nguyen, V.B. *et al*, *Tetrahedron Lett.*, 1986, **27**, 841 (*synth*)

6-Chloro-5-hexen-3-ol, 9CI C-80065



(*S,Z*)-*form*

$C_6H_{11}ClO$ M 134.605

(***S,Z***)-***form*** [90760-63-7]
Liq. $[\alpha]_D^{20}$ +9.2° (c, 9.15 in EtOH).

(±)-(***Z***)-***form*** [87921-54-8]
Liq.

Hoffmann, R.W. *et al*, *Chem. Ber.*, 1986, **119**, 1039, 2013 (*synth, pmr, cmr*)

2-Chloro-6-hydroxy-1,4-naphthoquinone C-80066

2-Chloro-6-hydroxy-1,4-naphthalenedione

[76665-65-1]

$C_{10}H_5ClO_3$ M 208.600
Cryst. (1,2-dichloroethane). Mp 229-230°.

Brisson, C. *et al*, *J. Org. Chem.*, 1981, **46**, 1810 (*synth, uv, ir, pmr*)
Boisvert, L. *et al*, *J. Org. Chem.*, 1988, **53**, 4052 (*synth, ir, uv, pmr*)

2-Chloro-7-hydroxy-1,4-naphthoquinone C-80067

2-Chloro-7-hydroxy-1,4-naphthalenedione

[69119-29-5]

$C_{10}H_5ClO_3$ M 208.600
Cryst. (dichloroethane). Mp 216-217°.

Brisson, C. *et al*, *J. Org. Chem.*, 1981, **46**, 1810 (*synth, uv, ir, pmr*)
Boisvert, L. *et al*, *J. Org. Chem.*, 1988, **53**, 4052 (*synth, ir, uv, pmr*)

Chloroiodomethane C-80068

[593-71-5]

$ClCH_2I$

CH_2ClI M 176.384
Versatile organic synthon. Liq. Bp 108-109° (104-105°) .

Miyano, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 2864 (*synth, pmr*)
Hahn, R.C., *J. Org. Chem.*, 1988, **53**, 1331 (*synth, bibl, use*)

1-Chloro-2-isocyanatoethane, 9CI C-80069

2-Chloroethyl isocyanate, 8CI

[1943-83-5]

$ClCH_2CH_2NCO$

C_3H_4ClNO M 105.523
Cryst. d_{20} 1.237. Fp 56°. Bp 135°, Bp_{16} 42°. n_D^{20} 1.4493.
▷ Corrosive, lachrymator.

Sadtler Standard Infrared Spectra, 23442, 42442 (*ir*)
Sadtler Standard NMR Spectra, 13504 (*pmr*)
Wenker, H., *J. Am. Chem. Soc.*, 1936, **58**, 2608 (*synth*)
Johnson, C.K., *J. Org. Chem.*, 1967, **32**, 1508 (*synth*)

Chloromethanol C-80070

[15454-33-8]

$ClCH_2OH$

CH_3ClO M 66.487

Ac: [625-56-9].
$C_3H_5ClO_2$ M 108.524
Alkylating agent. Oil. Bp_{748} 113-115°, Bp_5 28°. n_D^{20} 1.4102.

Chloroacetyl: [6135-23-5].
$C_3H_4Cl_2O_2$ M 142.969
Oil. Bp_{745} 130-132°, Bp_{21} 77.5°. n_D^{20} 1.4603.

Trichloroacetyl:
$C_3H_2Cl_4O_2$ M 211.858
Oil. d_4^{20} 1.60. Bp 170°, Bp_{10} 68°. n_D^{20} 1.5988.

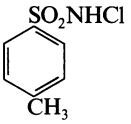
Benzoyl: [5335-05-7].
$C_8H_7ClO_2$ M 170.595
Oil. d_4^{25} 1.233. Bp_8 114-115°, Bp_6 98-99°. n_D^{25} 1.5328.

4-Methylbenzenesulfonyl: [117184-50-6].
$C_8H_9ClO_3S$ M 220.676
Oil. $Bp_{0.4}$ 99-101°.

Ulich, L.H. *et al*, *J. Am. Chem. Soc.*, 1921, **43**, 660 (*acetate, chloroacetate*)
Bavin, P.M.G., *Can. J. Chem.*, 1964, **42**, 704 (*acetate*)
Euranto, E.K. *et al*, *Acta Chem. Scand.*, 1966, **20**, 1273 (*trichloroacetate*)
Bodor, N. *et al*, *J. Med. Chem.*, 1980, **23**, 566 (*benzoate*)
Korhonen, I.O.O., *Org. Mass Spectrom.*, 1984, **19**, 34 (*ms*)
Hahn, R.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5783 (*synth, pmr, cmr*)

N-Chloro-4-methylbenzenesulfonamide C-80071

N-*Chloro*-p-*toluenesulfonamide*



$C_7H_8ClNO_2S$ M 205.664

Na Salt: [127-65-1]. *Chloramine T*
Oxidising agent. Cryst. + $3H_2O$ (H_2O or EtOH). Mp 176-180° (explodes). Explodes on melting. Respiratory irritant, may cause emphysema.

Heintzelman, R.W., *Synthesis*, 1976, 731 (*synth*)
Hutchins, M.G. *et al*, *J. Org. Chem.*, 1982, **47**, 4847 (*synth*)
Bremner, D.H., *Synth. Reagents*, 1985, **6**, 9 (*rev*)
Olmstead, M.P. *et al*, *Inorg. Chem.*, 1986, **25**, 4057 (*cryst struct*)

(Chloromethyl)pentafluorobenzene, 9CI C-80072

Pentafluorobenzyl chloride

[653-35-0]

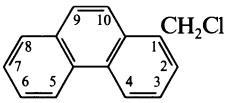
$(C_6F_5)CH_2Cl$

$C_7H_2ClF_5$ M 216.537
Liq. Bp 160-163°, Bp_{47} 80°.
▷ Slightly lachrymatory.

Barbour, A.K. *et al*, *J. Chem. Soc.*, 1961, 808 (*synth, ir*)

1-(Chloromethyl)phenanthrene C-80073

[20485-61-4]



$C_{15}H_{11}Cl$ M 226.705
Cryst. (pet. ether). Mp 89-90.5°.

Fierens, P.J.C. *et al*, *Helv. Chim. Acta*, 1955, **38**, 2005 (*synth*)

2-(Chloromethyl)phenanthrene C-80074

[885-21-2]

$C_{15}H_{11}Cl$ M 226.705
Cryst. (pet. ether). Mp 98°.

Fierens, P.J.C. *et al*, *Helv. Chim. Acta*, 1955, **38**, 2005 (*synth*)

3-(Chloromethyl)phenanthrene **C-80075**

[20485-60-3]

$C_{15}H_{11}Cl$ M 226.705
Cryst. (pet. ether). Mp 81-82°.

Fierens, P.J.C. *et al*, *Helv. Chim. Acta*, 1955, **38**, 2005 (*synth*)

4-(Chloromethyl)phenanthrene **C-80076**

[38021-49-7]

$C_{15}H_{11}Cl$ M 226.705
Cryst. (pet. ether). Mp 72-73°.

Fierens, P.J.C. *et al*, *Helv. Chim. Acta*, 1955, **38**, 2005 (*synth*)

9-(Chloromethyl)phenanthrene, 9CI **C-80077**

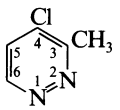
[951-05-3]

$C_{15}H_{11}Cl$ M 226.705
Cryst. (hexane). Mp 101-102°. Bp_1 186-188°.

Cook, J.W. *et al*, *J. Chem. Soc.*, 1935, 1319 (*synth*)
Tarbell, D.S. *et al*, *J. Am. Chem. Soc.*, 1943, **65**, 2149 (*synth*)
Fierens, P.J.C. *et al*, *Helv. Chim. Acta*, 1955, **38**, 2005 (*synth*)
Fernández, F. *et al*, *Synthesis*, 1988, 802 (*synth*)

4-Chloro-3-methylpyridazine, 9CI **C-80078**

[101346-01-4]



$C_5H_5ClN_2$ M 128.561

1-Oxide:
$C_5H_5ClN_2O$ M 144.560
Needles (EtOH). Mp 132.5-133°.

Ogata, M., *Chem. Pharm. Bull.*, 1963, **11**, 1511.

4-Chloro-5-methylpyridazine, 9CI **C-80079**

$C_5H_5ClN_2$ M 128.561

1-Oxide:
$C_5H_5ClN_2O$ M 144.560
Needles (C_6H_6/cyclohexane). Mp 61-62°.

Ogata, M., *Chem. Pharm. Bull.*, 1963, **11**, 1511.

2-Chloro-1-naphthylamine **C-80080**

2-Chloro-1-naphthalenamine, 9CI. 1-Amino-2-chloronaphthalene

[13711-39-2]

$C_{10}H_8ClN$ M 177.633
Needles. Mp 56°, Mp 60°. Steam-volatile.

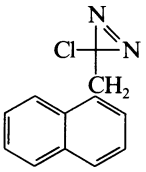
N-*Ac:* [13711-40-5].
$C_{12}H_{10}ClNO$ M 219.670
Needles (EtOH). Mp 195°.

N,N-*Di-Ac:*
$C_{14}H_{12}ClNO_2$ M 261.707
Prisms (EtOH aq.). Mp 88°.

Cleve, P.T., *Ber.*, 1887, **20**, 450.
Bowers, G.W., *J. Am. Chem. Soc.*, 1936, **58**, 1573.
Hodgson, H. *et al*, *J. Chem. Soc.*, 1942, 744; 1944, 538.
Stepanov, B.I., *Zh. Obshch. Khim.*, 1960, **30**, 2008.
Godfrey, K.E. *et al*, *J. Chem. Soc. C*, 1967, 400.

3-Chloro-3-(1-naphthylmethyl)diazirine **C-80081**

[112399-65-2]

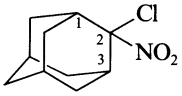


$C_{12}H_9ClN_2$ M 216.669
Cryst. (pentane). Mp 41°.

Linden, A. *et al*, *J. Org. Chem.*, 1988, **53**, 1085 (*synth, ir, uv, pmr, ms, cryst struct*)

2-Chloro-2-nitroadamantane **C-80082**

2-Chloro-2-nitrotricyclo[3.3.1.1^{3,7}]decane

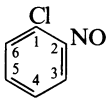


$C_{10}H_{14}ClNO_2$ M 215.679
Cryst. (EtOH aq.). Mp 200-201°.

Archibald, T.G. *et al*, *J. Org. Chem.*, 1988, **53**, 4645 (*synth, ir, pmr*)

1-Chloro-2-nitrosobenzene, 9CI **C-80083**

[932-33-2]



C_6H_4ClNO M 141.556
Needles (EtOH). Mp 56-57°.

Haworth, R.D. *et al*, *J. Chem. Soc.*, 1921, **119**, 768 (*synth*)

1-Chloro-3-nitrosobenzene, 9CI **C-80084**

[932-78-5]

C_6H_4ClNO M 141.556
Needles (C_6H_6). Mp 72°.

Haworth, R.D. *et al*, *J. Chem. Soc.*, 1921, **119**, 768 (*synth*)

1-Chloro-4-nitrosobenzene, 9CI **C-80085**

[932-98-9]

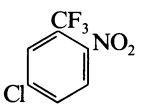
C_6H_4ClNO M 141.556
Cream cryst. (EtOH). Mp 130-140° dec. (92-93°). Cont. *ca.* 5% corresponding azoxy compd.

Ingold, C.K., *J. Chem. Soc.*, 1924, 87 (*synth*)
Defoin, A. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1199 (*synth, ir, pmr*)

4-Chloro-1-nitro-2-(trifluoromethyl) benzene **C-80086**

5-Chloro-α,α,α-trifluoro-2-nitrotoluene

[118-83-2]

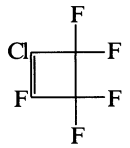


$C_7H_3ClF_3NO_2$ M 225.554
Pale yellow oil. Mp 21-22°. Bp 224°, Bp_{4-5} 86-87°.

Whalley, W.B., *J. Chem. Soc.*, 1949, 3016 (*synth*)
Newmark, R.A. *et al*, *Org. Magn. Reson.*, 1977, **9**, 589 (*C-13 nmr*)

1-Chloro-2,3,3,4,4-pentafluorocyclobutene, 9CI **C-80087**

[377-94-6]



C_4ClF_5 M 178.489
Bp 33-33.4°. n_D^{25} 1.3208.

Newmark, R.A. *et al*, *J. Magn. Reson.*, 1969, **1**, 418 (*F-19 nmr*)
Chia, L.S. *et al*, *Can. J. Chem.*, 1974, **52**, 3484 (*Cl-nqr*)
Bauer, G. *et al*, *Z. Naturforsch.*, *B*, 1979, **34**, 1249 (*synth*)

1-Chloro-1,1,3,3,3-pentafluoropropane, 9CI **C-80088**

[460-92-4]

$F_3CCH_2CClF_2$

$C_3H_2ClF_5$ M 168.493
Shows anaesthetic props. d_4^{20} 1.4372. Fp −107°. Bp 28.4°. n_D^{20} 1.2875.

[108662-83-5]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1946, **68**, 496 (*synth*)
Vorob'ev, V.N. *et al*, *Russ. J. Phys. Chem.*, 1974, **48**, 147 (*props*)
Di Paolo, T. *et al*, *J. Pharm. Sci.*, 1979, **68**, 39 (*pharmacol*)
Gachegov, Yu.N. *et al*, *Zh. Prikl. Spektrosk.*, 1979, **30**, 497 (*cryst struct*)

1-Chloro-2,2,3,3,3-pentafluoropropane **C-80089**

2,2,3,3,3-Pentafluoropropyl chloride

[422-02-6]

$F_3CCF_2CH_2Cl$

$C_3H_2ClF_5$ M 168.493
Shows anaesthetic props. d_4^{25} 1.395. Bp 25-27°. n_D^{20} 1.292.

McBee, E.T. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 3149 (*synth*)
Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1957, 2193 (*synth*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 1867 (*synth*)

1-Chloro-1,2,3,3,3-pentafluoro-1-propene, 9CI **C-80090**

[2804-49-1]

$F_3CCF{=}CFCl$

C_3ClF_5 M 166.478
Fp −156.8° to −159.6°. Bp 7.7-7.9°, Bp 8.4°. Mixt. of stereoisomers.

[14003-57-7, 14003-62-4, 89331-22-6]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 130 (*synth*)
Park, J.D. *et al*, *J. Org. Chem.*, 1958, **23**, 1169 (*synth*)
Fried, J.H. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 2078 (*synth*)
Paleta, O. *et al*, *Bull. Soc. Chim. Fr.*, 1986, 920 (*F nmr*)

4-Chloro-4-penten-1-ol **C-80091**

[1647-18-3]

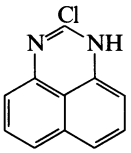
$H_2C{=}CClCH_2CH_2CH_2OH$

C_5H_9ClO M 120.578
Oil. $Bp_{3.1}$ 61.5-62.5°.

Wender, P.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2218 (*synth*, *ir*, *pmr*, *ms*)

2-Chloro-1*H*-perimidine **C-80092**

[30837-50-4]

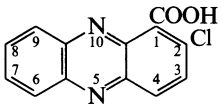


$C_{11}H_7ClN_2$ M 202.642
Pale green plates or yellow needles (Me_2CO). Mp 202-203.5° (194°).

Sachs, F., *Justus Liebigs Ann. Chem.*, 1909, **365**, 135 (*synth*)
Pozharskii, A.F. *et al*, *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1970, **6**, 1055 (*synth*)
Herbert, J.M. *et al*, *J. Med. Chem.*, 1987, **30**, 2081 (*synth*, *pmr*)

2-Chloro-1-phenazinecarboxylic acid, 9CI, 8CI **C-80093**

[106976-13-0]



$C_{13}H_7ClN_2O_2$ M 258.663
Cryst. (MeOH). Mp 247-249°.

Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

3-Chloro-1-phenazinecarboxylic acid, 9CI, 8CI **C-80094**

[103942-85-4]

$C_{13}H_7ClN_2O_2$ M 258.663
Cryst. (MeOH). Mp 255-257°.

Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

6-Chloro-1-phenazinecarboxylic acid, 9CI, 8CI **C-80095**

[103942-87-6]

$C_{13}H_7ClN_2O_2$ M 258.663
Cryst. (EtOH). Mp 310° dec.

Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

7-Chloro-1-phenazinecarboxylic acid, 9CI, 8CI **C-80096**

[103942-92-3]

$C_{13}H_7ClN_2O_2$ M 258.663
Cryst. (MeOH). Mp 274° dec.

Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

8-Chloro-1-phenazinecarboxylic acid, 9CI, 8CI **C-80097**

[103942-82-1]

$C_{13}H_7ClN_2O_2$ M 258.663
Cryst. (MeOH). Mp 286-289°.

N(5)-Oxide: [29137-34-6].
Cryst. Mp 116-117°.

Ger. Pat., 1 935 705, (1970); *CA*, **72**, 134173 (*oxide*)
Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

9-Chloro-1-phenazinecarboxylic acid, 9CI, 8CI **C-80098**

[103942-93-4]

$C_{13}H_7ClN_2O_2$ M 258.663
Cryst. (EtOH). Mp 272-273°.

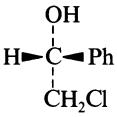
Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

2-Chloro-1-phenylethanol **C-80099**

Updated Entry replacing C-02052

α-(Chloromethyl)benzenemethanol, 9CI. α-Chloromethylbenzyl alcohol, 8CI. Styrene chlorohydrin. Phenylethylene chlorohydrin. β-Chloro-α-hydroxyethylbenzene. Chloromethylphenylcarbinol

[1674-30-2]



(*R*)-*form*

C_8H_9ClO M 156.611

(R)-form [56751-12-3]
Bp_{11} 119-120°. $[\alpha]_D^{25}$ −47.8° (c, 2.8 in hexane).

(S)-form
Liq. Bp_6 112-4°. $[\alpha]_D^{24}$ +49.6° (c, 2.81 in cyclohexane)(96.5% e.e.).

(±)-form
$d_4^{20.5}$ 1.16. Bp_6 110-111°. n_D^{20} 1.5400.

Ac: [79465-05-7].
$C_{10}H_{11}ClO_2$ M 198.648
Oil. Bp_3 101-104°.

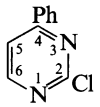
4-Nitrobenzoyl: Cryst. (EtOH). Mp 81°.

[829-23-2, 33942-01-7]

Emerson, W., *J. Am. Chem. Soc.*, 1945, **67**, 516 (*synth*)
Hanby, W.E. *et al*, *J. Chem. Soc.*, 1946, 114 (*synth*)
Sumrell, G. *et al*, *Can. J. Chem.*, 1964, **42**, 2896.
Gounelle, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 2815 (*ir*)
Hartgerink, J.W. *et al*, *Tetrahedron*, 1971, **27**, 4323.
Corey, E.J. *et al*, *J. Org. Chem.*, 1988, **53**, 2861 (*synth*)

2-Chloro-4-phenylpyrimidine, 9CI **C-80100**

[13036-50-5]



$C_{10}H_7ClN_2$ M 190.631
Cryst. (pet. ether). Mp 88.5-89.5°.

[56734-25-9]

Matsukawa, T. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1950, **70**, 134 (*synth*)
Lythgoe, B. *et al*, *J. Chem. Soc.*, 1951, 2323 (*synth*)
Kato, T. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 981 (*ms*)
Kroon, A.P. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1974, **93**, 325 (*use*)
Sedova, V.F. *et al*, *Khim. Geterotsikl. Soedin.*, 1977, **5**, 678 (*synth*)
Baram, S.G. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1982, 135; *ca*, **98**, 4208v (*cmr*)

2-Chloro-5-phenylpyrimidine, 9CI **C-80101**

[22536-62-5]

Cryst. (C_6H_6/pet. ether). Mp 124-128° (123°).

Brown, D.J. *et al*, *J. Chem. Soc. C*, 1970, 214 (*synth, pmr, uv*)
Allen, D.W. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1977, 621 (*synth*)
Ivanovskaya, L.Y. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1979, 71; *CA*, **90**, 203080g (*ms*)
Coppola, G.M. *et al*, *J. Heterocycl. Chem.*, 1980, **17**, 1479 (*synth, ir, pmr*)

4-Chloro-2-phenylpyrimidine, 9CI **C-80102**

[14790-42-2]

$C_{10}H_7ClN_2$ M 190.631
Cryst. (EtOH). Mp 74°.

[23149-84-0]

Van Meeteren, H.W. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1967, **86**, 15 (*synth*)
Geerts, J.P. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1973, **92**, 1232 (*pmr*)
Geerts, J.P. *et al*, *Org. Magn. Reson.*, 1975, **7**, 86 (*cmr*)
Ivanovskaya, L.Y. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1979, 71; *CA*, **90**, 203080g (*ms*)

4-Chloro-5-phenylpyrimidine, 9CI **C-80103**

[60122-80-7]

$C_{10}H_7ClN_2$ M 190.631
Cryst. (pet. ether). Mp 71-72°. Bp_{19} 156-158°.

Davies, W.H. *et al*, *J. Chem. Soc.*, 1945, 347 (*synth*)
Boarland, M.P.V. *et al*, *J. Chem. Soc.*, 1952, 3722 (*uv*)

4-Chloro-6-phenylpyrimidine, 9CI **C-80104**

[3435-26-5]

$C_{10}H_7ClN_2$ M 190.631
Solid. Mp 96-97.5°.

[39189-96-3, 40889-35-8]

van der Plas, H.C. *et al*, *Tetrahedron Lett.*, 1964, 2093 (*synth*)
De Valk, J. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1972, **91**, 1414 (*synth*)
Kato, T. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 981 (*ms*)
U.S. Pat., 3 908 012, (1975); *CA*, **84**, 59528r (*synth*)
Baram, S.G. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1982, 135; *CA*, **98**, 4208v (*cmr*)

5-Chloro-2-phenylpyrimidine, 9CI **C-80105**

[34771-50-1]

$C_{10}H_7ClN_2$ M 190.631
Small needles (EtOH). Mp 96°.

Kunckell, F. *et al*, *Chem. Ber.*, 1902, **35**, 3164 (*synth*)
Wagner, R.M. *et al*, *Chem. Ber.*, 1971, **104**, 2975 (*synth, pmr*)
Baram, S.G. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1983, 299 (*cmr*)

5-Chloro-4-phenylpyrimidine, 9CI **C-80106**

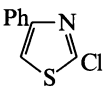
[72261-64-4]

$C_{10}H_7ClN_2$ M 190.631
Prisms (hexane). Mp 87.5-88.5°.

Yamanaka, H. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 3119 (*synth, pmr*)

2-Chloro-4-phenylthiazole, 9CI **C-80107**

[1826-23-9]



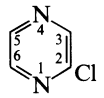
C_9H_6ClNS M 195.672
Cryst. (EtOH). Mp 53-54°.

B,MeFSO$_3$: Mp 138-139°.

B,EtBF$_4$: Mp 120-121°.

Bariana, D.S. *et al*, *J. Indian Chem. Soc.*, 1955, **32**, 427 (*synth*)
Vernin, G. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 2498 (*synth*)
Aune, J.P. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 2679 (*pmr*)
Sugimoto, H. *et al*, *J. Org. Chem.*, 1988, **53**, 2263 (*synth*)

2-Chloropyrazine C-80108



$C_4H_3ClN_2$ M 114.534
Liq. Bp_{26} 60.5°.

1-Oxide: [16025-16-4].
$C_4H_3ClN_2O$ M 130.533
Mp 140-146° (131-132°).

4-Oxide:
$C_4H_3ClN_2O$ M 130.533
Cryst. (EtOH aq.). Mp 95-96°.

Klein, B. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 2949 (*synth*)
Bernadi, L. *et al*, *Gazz. Chim. Ital.*, 1961, **91**, 1431 (*oxides*)
Klein, B. *et al*, *J. Org. Chem.*, 1963, **28**, 1682 (*synth, oxide, uv*)
Elisa, A.S. *et al*, *J. Heterocycl. Chem., USSR* (*Engl. Transl.*), 1967, **3**, 127 (*synth*)
Hashimoto, M. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1705 (*synth, pmr, uv*)

1-Chloro-2,3,3,3-tetrafluoro-1-propene, 9CI C-80109

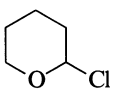
$F_3CCF{=}CHCl$

C_3HClF_4 M 148.487
Fumigant. Fp −115.8°. Bp 15.0°. Isomeric composition unknown.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1946, **68**, 496 (*synth*)

2-Chlorotetrahydro-2*H*-pyran, 9CI C-80110

[3136-02-5]



C_5H_9ClO M 120.578

(±)-*form*
Liq. Bp_{15} 44-45°, Bp_{12} 35-36°.

Booth, H. *et al*, *Tetrahedron*, 1987, **43**, 4699 (*synth, pmr, cmr, conformn*)

3-Chlorotetrahydro-2*H*-pyran C-80111

[6581-54-0]
C_5H_9ClO M 120.578

(±)-*form*
Liq. Bp 140-143°.

Crombie, L. *et al*, *J. Chem. Soc.*, 1956, 136 (*synth*)

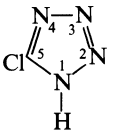
4-Chlorotetrahydro-2*H*-pyran C-80112

[1768-64-5]
C_5H_9ClO M 120.578
Liq. d_4^{20} 1.11. Bp_{12} 42°.

Hanschke, E., *Chem. Ber.*, 1955, **88**, 1053 (*synth*)

5-Chlorotetrazole C-80113

[55011-47-7]



1*H-form*

$CHClN_4$ M 104.498
Needles (C_6H_6). Mp 73°. pK_a 4.07.

Na salt: [96107-81-2].
Needles + $2H_2O$ (H_2O).
▷ Explodes when heated to 335°.

1H-form

*1-*tert*-Butyl:* [59772-99-5].
$C_5H_9ClN_4$ M 160.606
Cryst. (cyclohexane). Mp 114-115°.

1-Benzyl:
$C_8H_7ClN_4$ M 194.623
Mp 38°.

1-Ph:
$C_7H_5ClN_4$ M 180.596
Cryst. Mp 124°.

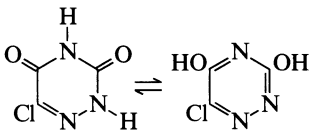
2H-form

*2-*tert*-Butyl:*
$C_5H_9ClN_4$ M 160.606
Oil. $Bp_{0.001}$ 25°.

Stollé, R. *et al*, *Chem. Ber.*, 1929, **62**, 1113 (*synth*)
Stollé, R. *et al*, *J. Prakt. Chem.*, 1932, **134**, 282 (*Phenyl*)
Lieber, E. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 1792 (*props*)
Henry, R.A. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 290 (*synth*)
Henry, R.A. *et al*, *J. Heterocycl. Chem.*, 1976, **13**, 391 (*tert*-Butyl)
Spear, R.J., *Aust. J. Chem.*, 1984, **37**, 2453 (*synth*)
Klich, M. *et al*, *Tetrahedron*, 1986, **42**, 2677 (*Benzyl, ir, pmr*)

6-Chloro-1,2,4-triazine-3,5(1*H*,3*H*)-dione, 9CI C-80114

6-Chloro-3,5-dihydroxy-1,2,4-triazine. 5-Chloro-6-azauracil



$C_3H_2ClN_3O_2$ M 147.520
Cryst. (H_2O). Mp 232-233° (225-227°). pK_a 5.80. Softens >200°.

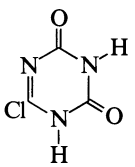
Benzylammonium salt: Cryst. (H_2O). Mp 232-233° (212-213°).

Chang, P.K., *J. Org. Chem.*, 1961, **26**, 1118 (*synth*)
Pískala, A. *et al*, *Collect. Czech. Chem. Commun.*, 1975, **40**, 2680 (*deriv*)
Farkaš, J., *Collect. Czech. Chem. Commun.*, 1983, **48**, 2676 (*deriv*)

6-Chloro-1,3,5-triazine-2,4(1*H*,3*H*)-dione, 9CI C-80115

2-Chloro-4,6-dihydroxy-1,3,5-triazine, 8CI

[69125-10-6]



$C_3H_2ClN_3O_2$ M 147.520

Known as salts.

Di-Me ether: [3140-73-6]. *2-Chloro-4,6-dimethoxy-1,3,5-triazine, 9CI*

$C_5H_6ClN_3O_2$ M 175.574

Coupling reagent for peptide synth. Cryst. (pet. ether). Mp 74.2-76.2°.

[32998-00-8, 54268-35-8, 67410-55-3]

Bovee, W.M.M.J. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1978, **97**, 107 (*synth, ir, pmr*)

1-Chloro-3,11-tridecadiene-5,7,9-triyn-2-ol C-80116

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH(OH)CH_2Cl$

$C_{13}H_{11}ClO$ M 218.682

(E,E)-form

Isol. from *Carthamus tinctorius*. Yellowish cryst (Et_2O/pet. ether). Mp 83°. $[\alpha]_{546}$ −3° (c, 0.33 in Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3433 (*isol, uv, ir, pmr, ord, struct*)

2-Chloro-3,11-tridecadiene-5,7,9-triyn-1-ol C-80117

[2060-58-4]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCHClCH_2OH$

$C_{13}H_{11}ClO$ M 218.682

(E,E)-form [16863-64-2]

Isol. from plants of the Asteraceae incl. *Centaurea*, *Gnaphalium*, and *Dicoma* spp. Has some pesticide/herbicide properties. Mp 68°. $[\alpha]_D^{20}$ −45.5° ($CHCl_3$), $[\alpha]_D^{20}$ −54.5° ($CHCl_3$).

Ac: [16982-47-1].

$C_{15}H_{13}ClO_2$ M 260.719

In *Centaurea*, *Dicoma*, *Coreopsis* spp. Cryst. (pet. ether). Mp 49°. $[\alpha]_D^{20}$ −10.3° (MeOH).

Bohlmann, F. *et al*, *Chem. Ber.*, 1958, **91**, 1642; 1961, **94**, 3179; 1967, **100**, 3201 (*isol, ir, uv*)
Anderson, A.B. *et al*, *Phytochemistry*, 1977, **16**, 1829 (*isol*)
Bohlmann, F. *et al*, *Phytochemistry*, 1978, **17**, 570; 1980, **19**, 71; 1983, **22**, 2858 (*isol*)
Jente, R. *et al*, *Phytochemistry*, 1979, **18**, 829 (*pmr*)
Picman, A.K. *et al*, *J. Chromatogr.*, 1980, **189**, 187 (*chromatog*)
Arnason, T. *et al*, *Can. J. Bot.*, 1981, **59**, 54; *CA*, **94**, 169071a (*tox*)
McLacklan, D. *et al*, *Biochem. Syst. Ecol.*, 1986, **14**, 17; *CA*, **105**, 1789n.

1-Chloro-2,3,3-trifluorocyclopropene, 9CI C-80118

[24921-89-9]

C_3ClF_3 M 128.481

Bp 20-21°, Bp 28°.

Camaggi, G. *et al*, *J. Chem. Soc. C*, 1970, 178 (*synth, ir, F-19 nmr, ms*)
Law, D.C.F. *et al*, *J. Org. Chem.*, 1973, **38**, 768 (*synth, ir, F-19 nmr, ms*)

1-Chloro-1,1,2-trifluoro-2-iodoethane, 9CI C-80119

[354-26-7]

$F_2CClCHFI$

C_2HClF_3I M 244.382

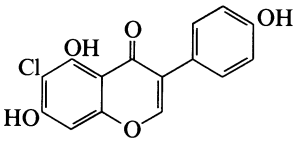
Shows anaesthetic props. d_4^{20} 2.181. Bp 82-83°. n_D^{20} 1.433.

Griffin, C.E. *et al*, *J. Chem. Soc.*, 1960, 1398 (*synth, uv*)
Norris, R.D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 182 (*F-19 nmr*)
Buchet, R. *et al*, *Biophys. Chem.*, 1985, **22**, 249 (*use*)

6-Chloro-4′,5,7-trihydroxyisoflavone C-80120

6-Chloro-5,7-dihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 6-Chlorogenistein

[64545-64-8]



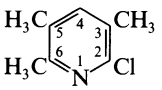
$C_{15}H_9ClO_5$ M 304.686

Metab. of *Streptomyces griseus*. All isolations of isoflavonoids from microorganisms are considered dubious. Prob. an artifact derived from the soybean medium.

König, W.A. *et al*, *Helv. Chim. Acta*, 1977, **60**, 2071 (*isol, ir, pmr, ms, struct*)

2-Chloro-3,5,6-trimethylpyridine C-80121

[121767-77-9]



$C_8H_{10}ClN$ M 155.626

Mp 60°.

Mittelbach, M. *et al*, *Acta Chem. Scand.*, *Ser. B*, 1988, **42**, 524 (*synth, pmr*)

3-Chloro-2,4,6-trimethylpyridine C-80122

$C_8H_{10}ClN$ M 155.626

Mp 150-151°. Bp 190-192°.

Batkowski, T. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1962, **36**, 51 (*synth*)

4-Chloro-2,3,5-trimethylpyridine, 9CI C-80123

[109371-18-8]

$C_8H_{10}ClN$ M 155.626

Oil.

N-Oxide:

$C_8H_{10}ClNO$ M 171.626

Mp 148°.

Japan. Pat., 6 272 666, (1987); *CA*, **107**, 96598a (*synth*)
Joiner, K.A. *et al*, *Tetrahedron Lett.*, 1987, **28**, 3733 (*use*)
Mittelbach, M. *et al*, *Acta Chem. Scand.*, *Ser. B*, 1988, **42**, 524 (*synth, pmr*)

Cholesta-7,22-diene-3,6-diol C-80124

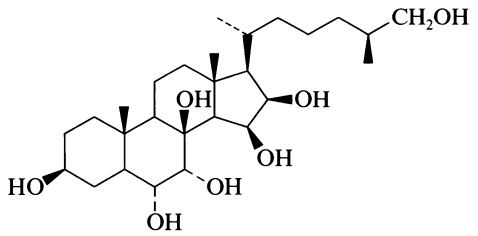
$C_{27}H_{44}O_2$ M 400.643

(3β,5α,6α,22E)-form

Constit. of *Spongionella gracillis*. Cryst. (MeOH/pet. ether). Mp 172-174°.

Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol, pmr*)

Cholestane-3,6,7,8,15,16,26-heptol C-80125



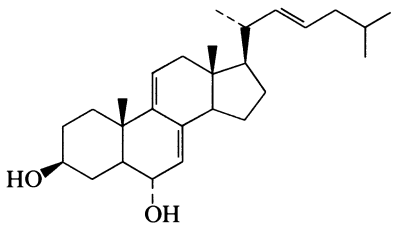
$C_{27}H_{48}O_7$ M 484.672

(3β,5α,6α,7α,8β,15β,16β,25S)-form

Constit. of *Pyncopodia helianthoides*. $[\alpha]_D$ +16°.

Bruno, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1022.

Cholesta-7,9(11),22-triene-3,6-diol C-80126



$C_{27}H_{42}O_2$ M 398.628

(3β,5α,6α,22E)-form

Constit. of *Spongionella gracilis*. Cryst. (MeOH/pet. ether). Mp 184-186°.

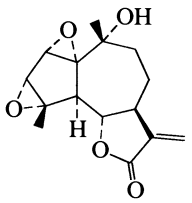
Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol*, *pmr*)

Chrysartemin A C-80127

Updated Entry replacing C-02435

Canin

[24959-84-0]



$C_{15}H_{18}O_5$ M 278.304

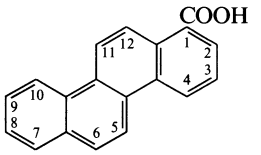
There is considerable confusion in the literature concerning the structure of this compound. Constit. of *Chrysanthemum parthenium*, *C. morifolium*, *Artemisia mexicana*, *A. klotzchiana*and *Tanacetum parthenium*. Cryst. (Me_2CO). Mp 250°. $[\alpha]_D^{20}$ −13.4° (c, 0.35 in $CHCl_3$). The structs. of closely related compds. Chrysartemin B and Artecanin require clarification at present.

[29431-83-2, 29431-84-3]

Begley, M.J. *et al*, *Phytochemistry*, 1989, **28**, 940 (*isol*, *cryst struct*, *bibl*)

1-Chrysenecarboxylic acid C-80128

[87717-16-6]



$C_{19}H_{12}O_2$ M 272.303

Mp >350°.

Me ester: [90340-68-4].

$C_{20}H_{14}O_2$ M 286.329

Cryst. (Me_2CO). Mp 175-176°.

Nitrile: [68723-52-4]. *1-Cyanochrysene*

$C_{19}H_{11}N$ M 253.303

Cryst. (C_6H_6/EtOH). Mp 228-229°.

Gore, P.H. *et al*, *Synthesis*, 1978, 773 (*synth*, *deriv*, *ir*, *pmr*)
Gore, P.H. *et al*, *Synth. Commun.*, 1980, **10**, 319 (*synth*, *deriv*)
Jones, A.J. *et al*, *Aust. J. Chem.*, 1984, **37**, 561 (*synth*, *deriv*, *pmr*, *ms*)

2-Chrysenecarboxylic acid C-80129

[96403-26-8]

$C_{19}H_{12}O_2$ M 272.303

Pale yellow needles (dioxan). Mp 325-327° dec.

Me ester:

$C_{20}H_{14}O_2$ M 286.329

Pale yellow plates (C_6H_6). Mp 219°.

Carruthers, W. *et al*, *J. Chem. Soc.*, 1953, 3486; 1954, 2047.

3-Chrysenecarboxylic acid C-80130

[96403-20-2]

$C_{19}H_{12}O_2$ M 272.303

Pale yellow needles (dioxan aq.). Mp 295° dec.

Me ester:

$C_{20}H_{14}O_2$ M 286.329

Plates. Mp 146-147°.

Nitrile: [36288-23-0]. *3-Cyanochrysene*

$C_{19}H_{11}N$ M 253.303

Cryst. (EtOH). Mp 200-201°.

Carruthers, W., *J. Chem. Soc.*, 1953, 3486 (*synth*, *deriv*)
Leznoff, C.C. *et al*, *Can. J. Chem.*, 1972, **50**, 528 (*synth*, *deriv*, *uv*, *pmr*)
Gore, P.H. *et al*, *Synthesis*, 1978, 773 (*synth*, *deriv*, *ir*, *pmr*)

5-Chrysenecarboxylic acid C-80131

Updated Entry replacing C-40154

[68723-48-8]

$C_{19}H_{12}O_2$ M 272.303

Buff needles (C_6H_6/Me_2CO). Mp 225-226° (212-224°).

Me ester: [71431-97-5].

$C_{20}H_{14}O_2$ M 286.329

Prisms (C_6H_6). Mp 159-160°.

Nitrile: [68723-47-7]. *5-Cyanochrysene*

$C_{19}H_{11}N$ M 253.303

Cryst. (MeOH). Mp 165.5°.

Fieser, L.F. *et al*, *J. Am. Chem. Soc.*, 1940, **60**, 1211 (*synth*)
Gore, P.H. *et al*, *Synthesis*, 1978, 773 (*synth*, *deriv*, *ir*, *pmr*)
Gore, P.H. *et al*, *Tetrahedron*, 1979, **35**, 2927 (*nitrile*)
Lee-Ruff, E. *et al*, *J. Org. Chem.*, 1984, **49**, 553 (*synth*)

6-Chrysenecarboxylic acid C-80132

[95646-96-1]

$C_{19}H_{12}O_2$ M 272.303
Needles (dioxan). Mp 314°.

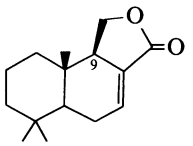
Me ester: [99762-96-6].
$C_{20}H_{14}O_2$ M 286.329
Needles (EtOH). Mp 148°.

Nitrile: [68723-50-2]. *6-Cyanochrysene*
$C_{19}H_{11}N$ M 253.303
Cryst. (C_6H_6/EtOH).

Dewar, M.J.S. *et al*, *J. Chem. Soc.*, 1957, 2946 (*synth, deriv*)
Gore, P.H. *et al*, *Synthesis*, 1978, 773 (*synth, deriv, ir, pmr*)
Gore, P.H. *et al*, *Tetrahedron*, 1979, **35**, 2927 (*synth, deriv*)

Cinnamolide C-80133

Updated Entry replacing C-02480
[23599-47-5]



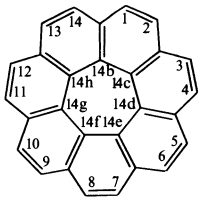
$C_{15}H_{22}O_2$ M 234.338
Constit. of *Cinnamosa fragrans*. Cryst. Mp 125-126°. $[\alpha]_D^{20}$ −29.4° (c, 1 in $CHCl_3$).

9α-Hydroxy: ***9α-Hydroxycinnamolide***
$C_{15}H_{22}O_3$ M 250.337
Constit. of *Canella winterana*. Cryst. Mp 150-155°. $[\alpha]_D$ −10° (c, 0.44 in $CHCl_3$).

Suzuki, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 1268 (*synth*)
Yamagawa, H. *et al*, *Synthesis*, 1970, 257 (*synth*)
Nakanishi, K. *et al*, *Isr. J. Chem.*, 1977, **16**, 28 (*isol*)
Kioy, D. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 174 (*isol, deriv, pmr, cmr*)

[7]Circulene C-80134

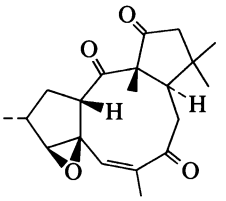
Updated Entry replacing C-30165
Dinaphtho[*2,1,8,7*-ghij:*2′,2′,8′,7′*-nopq]*pleiadene*, *9CI*
[76276-09-0]



$C_{28}H_{14}$ M 350.419
Yellow plates. Mp 295-296°.

Yamamoto, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3578 (*synth, uv, ir, pmr, cmr, ms, cryst struct*)

Citlalitrione C-80135

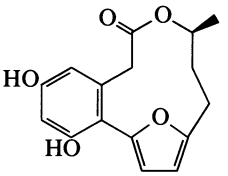


$C_{20}H_{26}O_4$ M 330.423
Constit. of *Jatropha dioica* var. *sessiliflora*. Cryst. (MeOH/hexane). Mp 194-196°. $[\alpha]_D$ −146° (c, 7.5 in $CHCl_3$).

Villarreal, A.M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 749 (*isol, cryst struct*)

Citreofuran C-80136

[122400-13-9]

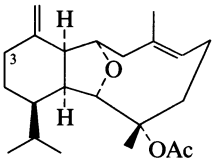


$C_{16}H_{16}O_5$ M 288.299
Metab. of hybrid strain of *Penicillium citreo-viride B.* Cryst. Mp 203-205°. $[\alpha]_D^{27}$ +112° (c, 0.18 in EtOH).

Lai, S. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2241.

Cladiellin C-80137

Updated Entry replacing C-02522
[66873-35-6]



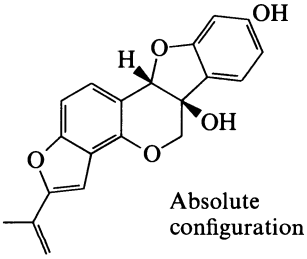
$C_{22}H_{34}O_3$ M 346.509
Constit. of *Cladiella* spp.

Δ^3-*Isomer*, O-*de-Ac:*
$C_{20}H_{32}O_2$ M 304.472
Constit. of *C.* spp. Cryst. Mp 48-52°. $[\alpha]_D$ −22.7° (c, 0.3 in $CHCl_3$).

Kazlauskas, R. *et al*, *Tetrahedron Lett.*, 1977, 4643 (*isol*)
Hochlowski, J.E. *et al*, *Tetrahedron Lett.*, 1980, 4055 (*isol, deriv*)

Clandestacarpin C-80138

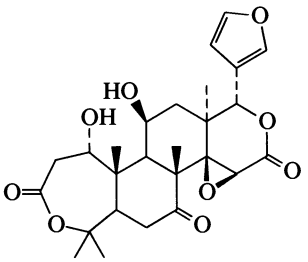
[79002-16-7]



$C_{20}H_{16}O_5$ M 336.343
Phytoalexin from fungus-infected leaves of *Glycine clandestina*, *G. tabacina* and *G. tomentella*. Phytoalexin.

Lyne, R.L. *et al*, *Tetrahedron Lett.*, 1981, 2483 (*isol, struct, abs config*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*isol*)

Clausenarin C-80139

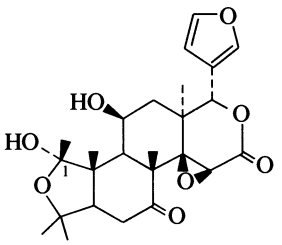


$C_{26}H_{32}O_9$ M 488.533
Constit. of *Clausena anisata*. Cryst. (DMSO aq.). Mp 293-294°. $[\alpha]_D^{25}$ −87.5° (c, 1.04 in Me_2CO).

Ngadjui, B.T. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 832 (*isol, pmr, cmr*)

Clausenolide C-80140

Updated Entry replacing C-02534
[71899-58-6]

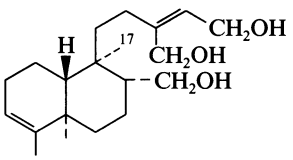


$C_{25}H_{32}O_8$ M 460.523
Constit. of *Clausena heptaphylla*. Cryst. Mp 150°. $[\alpha]_D^{27}$ −70.7° (c, 1 in $CHCl_3$).

1-Et ether:
$C_{27}H_{36}O_8$ M 488.577
Constit. of *C. anisata*. Cryst. (Et_2O). Mp 134-135°. $[\alpha]_D$ −63.5° (c, 1.02 in $CHCl_3$).

Chakraborty, D.P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 246 (*isol*)
Ngadjui, B.T. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 832 (*isol, pmr, cmr*)

ent-3,13-Clerodadiene-15,16,17-triol C-80141



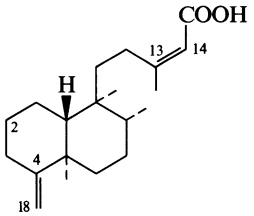
$C_{20}H_{34}O_3$ M 322.487
Constit. of *Baccharis boliviensis*.

17-O-β-Xylopyranoside:
$C_{25}H_{40}O_8$ M 468.586
Constit. of *B. boliviensis*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

ent-4(18),-13-Clerodadien-15-oic acid C-80142

[120552-37-6]



$C_{20}H_{32}O_2$ M 304.472
Constit. of *Ageratina ixiocladon*.

4α,18-Epoxide: [120552-39-8]. **ent-*4β,18-Epoxy-13-cleroden-15-oic acid***
$C_{20}H_{32}O_3$ M 320.471
Constit. of *A. ixiocladon*.

4β,18-Epoxide: [120662-27-3]. **ent-*4α,18-Epoxy-13-cleroden-15-oic acid***
$C_{20}H_{32}O_3$ M 320.471
Constit. of *A. ixiocladon*.

13,14-Dihydro: [120552-38-7]. **ent-*4(18)-Cleroden-15-oic acid***
$C_{20}H_{34}O_2$ M 306.487
Constit. of *A. ixiocladon*.

13,14-Dihydro, 4α,18-epoxide: [120552-40-1]. **ent-*4β,18-Epoxy-15-clerodanoic acid***
$C_{20}H_{34}O_3$ M 322.487
Constit. of *A. ixiocladon*.

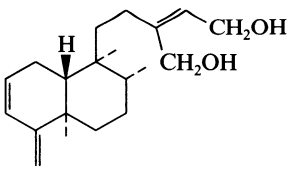
13,14-Dihydro, 4β,18-epoxide: [120662-28-4]. **ent-*4α,18-Epoxy-15-clerodanoic acid***
$C_{20}H_{34}O_3$ M 322.487
Constit. of *A. ixiocladon*.

4,18-Dihydro,4α-hydroxy: [120662-29-5]. **ent-*4β-Hydroxy-13-cleroden-15-oic acid***
$C_{20}H_{34}O_3$ M 322.487
Constit. of *A. ixiocladon*.

$\Delta^{3,4}$-*Isomer, 2-oxo:* [120662-30-8]. **ent-*2-oxo-3,13-clerodadien-15-oic acid***
$C_{20}H_{30}O_3$ M 318.455
Constit. of *A. ixiocladon*.

Tanayo-Castillo, G. *et al*, *Phytochemistry*, 1989, **28**, 139.

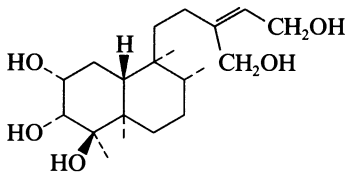
ent-2,4(18),13-Clerodatriene-15,16-diol C-80143



$C_{20}H_{32}O_2$ M 304.472
Constit. of *Baccharis boliviensis*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

ent-13-Clerodene-2β,3β,4α,15,16-pentol C-80144



$C_{20}H_{36}O_5$ M 356.501
Constit. of *Baccharis boliviensis*.

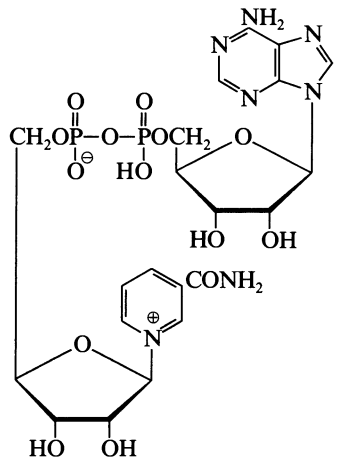
Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

Coenzyme I, 8CI C-80145

Updated Entry replacing C-02663

Adenosine 5′-(trihydrogen diphosphate) (5′→5′) ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium hydroxide inner salt, 9CI. Nicotinamide adenine dinucleotide. ***Nadide,*** **BAN, USAN, INN.** *Codehydrase I. Codehydrogenase I. Cozymase. Diphosphopyridine nucleotide. Enzopride. DPN. NAD. NSC 20272. Co I. NAD⁺*

[53-84-9]



$C_{21}H_{27}N_7O_{14}P_2$ M 663.430
Isol. from bakers' yeast. Antagonist to alcohol and narcotic analgesics. Biological hydrogen acceptor. Hygroscopic powder. Sol. H_2O. λ_{max} 260 (ϵ 17.6 × 10^6) (H_2O), 340 nm (6.2 × 10^6)(reduced form). Forms a complex with alkaline cyanide which may be used for its estimation. Stable for weeks in cold neutral soln. Less stable in acid soln., rapidly dec. by alkali.

▷ UU3450000.

Dihydro: [58-68-4]. *Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 1,4-dihydro-1-β-D-ribofuranosyl-3-pyridinecarboxamide, 9CI. NADH*
$C_{21}H_{29}N_7O_{14}P_2$ M 665.446
Reduced form of Coenzyme I in biological systems.

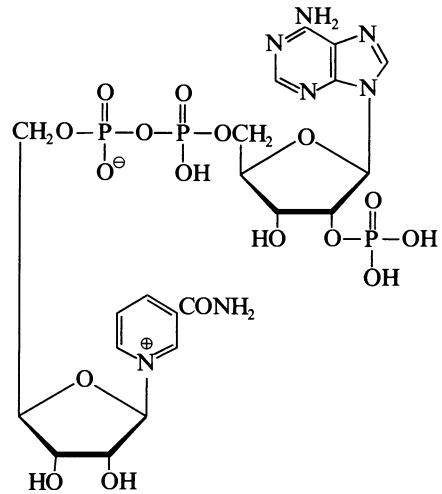
Biochem. Prep., 1949, **1**, 28 (*isol*)
Biochem. Prep., 1953, **3**, 20 (*isol, synth*)
Hughes, N.A. *et al*, *J. Chem. Soc.*, 1957, 3733 (*synth*)
Lemieux, R.U. *et al*, *Can. J. Chem.*, 1963, **41**, 889 (*stereochem*)
Biochem. Prep., 1966, **11**, 84 (*purifn*)
Sarma, R.H. *et al*, *Biochemistry*, 1970, **9**, 557 (*conformn, pmr*)
Blumenstein, M. *et al*, *Biochemistry*, 1973, **12**, 3585 (*cmr*)
Nishizuka, Y. *et al*, *Method. Chim.*, 1977, **11**, 84 (*rev*)
Walsh, C., *Annu. Rev. Biochem.*, 1978, **47**, 881 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 12991.
Kemal, C., *Comprehensive Heterocyclic Chemistry*, Katritzky A.R. and Rees C.W., Eds., Pergamon, 1984, **1**, 247 (*rev, bibl*)
Walt, D.R. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 234 (*synth*)

Coenzyme II, 9CI, 8CI C-80146

Updated Entry replacing C-02664

Adenosine 5′-(trihydrogen diphosphate) 2′-(dihydrogen phosphate) (5′→5′) ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium hydroxide inner salt, 9CI. Nicotinamide adenine dinucleotide phosphate. Codehydrase II. Codehydrogenase II. Nadifosfate. Phosphocozymase. Triphosphopyridine nucleotide. NADP. TPN. NADP⁺

[53-59-8]



$C_{21}H_{28}N_7O_{17}P_3$ M 743.410
Wide occurrence in living matter, particularly in the liver and in red blood corpuscles, mainly in the reduced form. A component of vitamin B_2 complex. Hydrogen carrier in biochemical redox systems. In the hexose monophosphoric acid system it is reduced to Dihydrocoenzyme II and reoxid. in the presence of flavoproteins. Greyish-white powder. Sol. H_2O. pK_{a1} 3.9, pK_{a2} 6.1. λ_{max} 260 (ϵ 18 × 10^6)(H_2O), 340 nm (ϵ 6.2 × 10^6)(reduced form).

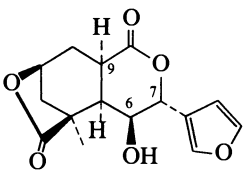
Mono-Na salt: Cryst. + H_2O. Mp 175-178° dec.

Dihydro: [53-57-6]. *NADPH*
$C_{21}H_{30}N_7O_{17}P_3$ M 745.426
Reduced form of Coenzyme II in biological systems.

Todd, A.R., *J. Chem. Soc.*, 1941, 427 (*rev*)
Lepage, G.A., *J. Biol. Chem.*, 1949, **180**, 775 (*isol*)
Biochem. Prep., 1953, **3**, 24 (*isol, synth*)
Sund, R., *The Pyridine Nucleotide Coenzymes*, in *Biological Oxidations*, (Singer, T.,Ed.), Interscience, N.Y., 1968, 603 (*rev*)
Blumenstein, M. *et al*, *Biochemistry*, 1973, **12**, 3585 (*cmr*)
Sarma, R.H. *et al*, *Can. J. Chem.*, 1973, **51**, 1843 (*nmr*)
Nishizuka, Y., *Method. Chim.*, 1977, **11**, 84 (*rev*)
Wood, H.C.S., *Compr. Org. Chem.*, Eds., Barton D.H.R. and Ollis, W.D., Pergamon, 1979, **5**, 490 (*rev, bibl*)
Walt, D.R. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 234 (*synth*)

Collybolidol C-80147

Updated Entry replacing I-00948



Absolute configuration

$C_{15}H_{16}O_6$ M 292.288
Parent compd. unknown. Hydrol. of Collybolide causes opening of the lactone ring.

O-*Benzoyl:* [33340-30-6]. ***Collybolide***

$C_{22}H_{20}O_7$ M 396.396
Constit. of the basidiomycete *Collybia maculata*. Cryst. (EtOH). Mp 210°. $[\alpha]_D$ +17° ($CHCl_3$).

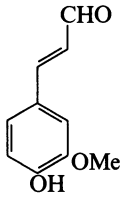
9-Epimer, O-benzoyl: [31199-75-4]. ***Isocollybolide***
$C_{22}H_{20}O_7$ M 396.396
Constit. of *C. maculata*. Mp 193°. $[\alpha]_D$ −17° (c, 1.7 in $CHCl_3$).

7,9-Diepimer, 6-deoxy: [106794-13-2]. ***Deoxycollybolidol***
$C_{15}H_{16}O_5$ M 276.288
Constit. of *C. peronata*. Cryst. (EtOAc/hexane). Mp 189-190°. $[\alpha]_D$ +21° (c, 0.1 in $CHCl_3$).

Pascard-Billy, C., *Acta Crystallogr., Sect. C*, 1972, **28**, 331 (*cryst struct, Isocollybolide*)
Bui, A.M. *et al*, *Tetrahedron*, 1974, **30**, 1327 (*isol, pmr, cmr, uv, struct*)
Fogedal, M. *et al*, *Phytochemistry*, 1986, **25**, 2661 (*Deoxycollybolidol*)

Coniferaldehyde C-80148

3-(4-Hydroxy-3-methoxyphenyl)-2-propenal, 9CI. 4-Hydroxy-3-methoxycinnamaldehyde. Ferulaldehyde. Hadromal
[458-36-6]



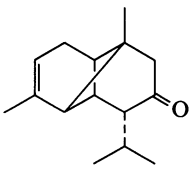
$C_{10}H_{10}O_3$ M 178.187
(E)-form [20649-42-7]
Occurs in wood, free and as component of lignin. Found extensively in brandies etc. as leachingprod. from wood. Light-yellow needles (pet. ether). Mp 84°.

2,4-Dinitrophenylhydrazene: Mp 265-266°.

Tiemann, F., *Ber.*, 1885, **18**, 3481 (*synth*)
Adler, E. *et al*, *Acta Chem. Scand.*, 1948, **2**, 839 (*isol*)
Black, R.A. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 5344 (*isol, uv*)
Nakanura, Y. *et al*, *CA*, 1977, **86**, 139537z (*synth*)
Liptaj, T. *et al*, *Collect. Czech. Chem. Commun.*, 1980, **45**, 33 (*pmr*)
Kutsuki, H. *et al*, *CA*, 1981, **95**, 132414j (*synth*)

2-Copaen-8-one C-80149

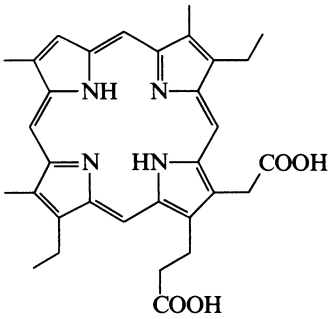
α-Copaen-8-one



$C_{15}H_{22}O$ M 218.338
Constit. of *Neomirandea guevarii*. Oil. $[\alpha]_D^{24}$ +14° (c, 0.53 in $CHCl_3$).

Tamayo-Castillo, G. *et al*, *Phytochemistry*, 1989, **28**, 938.

Corallistin A C-80150

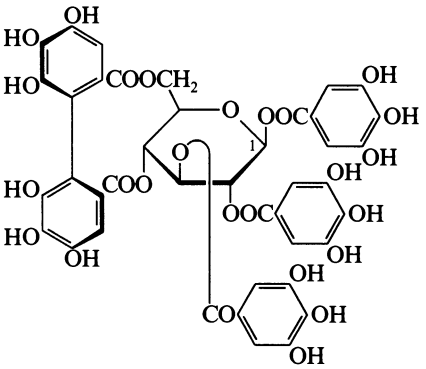


$C_{32}H_{34}N_4O_4$ M 538.645
Isol. from a Coral Sea desmosponge *Corallistes* sp. Rare example of a free porphyrin from a natural organism.

D'Ambrosio, M. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1451 (*isol, uv, pmr, cmr, struct*)

Cornus-tannin 2 C-80151

1,2,3-Tri-O-galloyl-4,6-O-hexahydroxydiphenoylglucose
[58970-75-5]



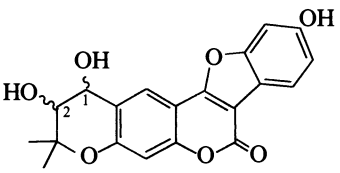
$C_{41}H_{30}O_{25}$ M 922.673
Isol. from fruits of *Cornus officinalis* and from *Tellima grandiflora*.

1-O-Degalloyl: [30737-92-9]. ***Cornus-tannin 3***
$C_{34}H_{26}O_{22}$ M 786.566
Isol. from fruits of *C. officinalis* and from *T. grandiflora*.

Wilkins, C.K. *et al*, *Phytochemistry*, 1976, **15**, 211.
Okuda, T. *et al*, *Heterocycles*, 1981, **16**, 1321.

Corylidin C-80152

Updated Entry replacing C-20231
[63109-31-9]



$C_{20}H_{16}O_7$ M 368.342
CA numbering shown. Constit. of the fruits of *Psoralea corylifolia*. Needles (EtOH/Me_2CO). Mp 349-351°.

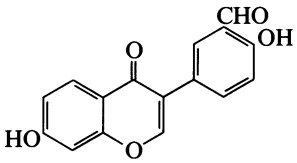
1,2-Dideoxy: [3564-61-2]. ***Isopsoralidin***
$C_{20}H_{16}O_5$ M 336.343
Isol. from seeds of *P. corylifolia*. Cryst. (MeOH). Mp 284-287°. Violet fluor in EtOH soln.

Jain, A.C. *et al*, *Indian J. Chem.*, 1974, **12**, 659 (*Isopsoralidin*)
Gupta, G.K. *et al*, *Phytochemistry*, 1977, **16**, 403 (*isol*)

Corylinal C-80153

*2-Hydroxy-5-(7-hydroxy-4-oxo-4*H*-1-benzopyran-3-yl)benzyaldehyde, 9CI. 3′-Formyl-4′,7-dihydroxyisoflavone*

[65615-46-5]



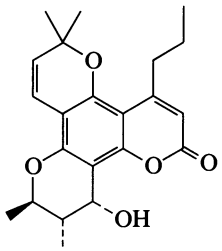
$C_{16}H_{10}O_5$ M 282.252

Isol. from seeds of *Psoralea corylifolia*. Isol. as Me ether after methylation.

7-Me ether: Needles (MeOH). Mp 223-224°.

Gupta, G.K. *et al*, *Phytochemistry*, 1978, **17**, 164.

Costatolide C-80154



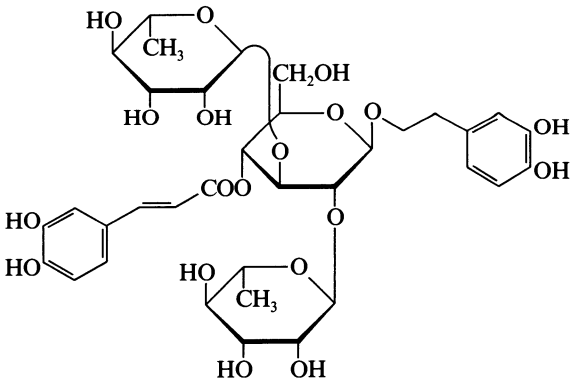
$C_{22}H_{26}O_5$ M 370.444

Isol. from resin of *Calophyllum costatum*. Cryst. (C_6H_6). Mp 181-182°. $[\alpha]_D^{25}$ −19.9° (c, 0.42 in $CHCl_3$), $[\alpha]_D^{25}$ −50.4° (c, 1.55 in Me_2CO).

Stout, G.H. *et al*, *J. Org. Chem.*, 1964, **29**, 3604 (*isol, uv, ir, pmr, ms, struct*)

Crassifolioside C-80155

[120693-47-2]



$C_{35}H_{46}O_{19}$ M 770.737

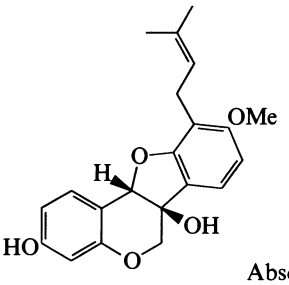
Constit. of *Plantago crassifolia*. Pale yellow amorph. powder. $[\alpha]_D^{20}$ −110.9° (c, 0.32 in MeOH).

Andary, C. *et al*, *Phytochemistry*, 1989, **28**, 288.

Cristacarpin C-80156

*9-Methoxy-10-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-c][1]benzopyran-3,6-(11*a*H)-diol, 9CI. 3,6a-Dihydroxy-9-methoxy-10-prenylpterocarpan. Erythrabyssin I*

[74515-47-2]



Absolute configuration

$C_{21}H_{22}O_5$ M 354.402

Isol. from *Erythrina abyssinica*, *E. crista-galli*, *E. sandwicensis* and *Psophocarpus tetragonolobus*. Phytoalexin. $[\alpha]_D$ −220° (c, 0.02 in MeOH).

O-*De-Me:* [74515-45-0]. ***Sandwicarpin***

$C_{20}H_{20}O_5$ M 340.375

Isol. from leaves of *E. sandwicensis*. Phytoalexin. $[\alpha]_D$ −278° (MeOH).

Ingham, J.L. *et al*, *Phytochemistry*, 1980, **19**, 1203 (*isol, uv, ms, struct, abs config*)

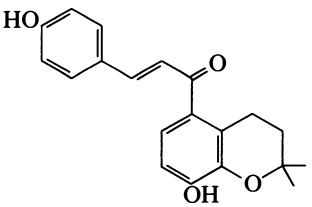
Ingham, J.L., *Z. Naturforsch.*, *C*, 1980, **35**, 384 (*Sandwicarpin*)

Kamat, V.S. *et al*, *Heterocycles*, 1981, **15**, 1163 (*isol, uv, cd, abs config*)

Crotmadine C-80157

Updated Entry replacing C-30199

[92662-86-7]



$C_{20}H_{20}O_4$ M 324.376

Constit. of *Crotalaria madurensis*. Cryst. ($CHCl_3$/MeOH). Mp 191°.

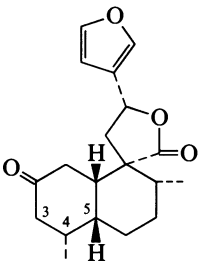
Bhakuni, D.S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1984, **47**, 585 (*isol*)

Malhotra, S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 578 (*struct*)

Crotonin C-80158

Updated Entry replacing C-30201

[17633-81-7]



$C_{19}H_{24}O_4$ M 316.396

Constit. of *Croton lucidus*. Cryst. (EtOAc/hexane). Mp 148-149°. $[\alpha]_D$ −1.4° ($CHCl_3$).

5-Epimer: **t-*Crotonin***

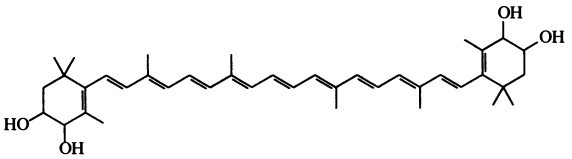
$C_{19}H_{24}O_4$ M 316.396
Constit. of *C. cajucara*. Needles. Mp 131-132°. $[\alpha]_D$ +2.3° (c, 3.29 in $CHCl_3$).

5-Epimer, 3,4-didehydro: ***t-Dehydrocrotonin***
$C_{19}H_{22}O_4$ M 314.380
Constit. of *C. cajucara*. Needles. Mp 138.5-140.5°. $[\alpha]_D$ +11.9° (c, 0.3 in $CHCl_3$).

Chan, W.R. *et al*, *J. Chem. Soc. C*, 1968, 2781 (*isol*)
Blount, J.F. *et al*, *J. Chem. Res.* (*S*), 1984, 114 (*cryst struct*)
Itokawa, H. *et al*, *Phytochemistry*, 1989, **28**, 1667 (*isol*)

Crustaxanthin C-80159

β,β-Carotene-3,3′,4,4′-tetrol
[6094-35-5]



$C_{40}H_{56}O_4$ M 600.880
Isol. from the crustacean *Arctodiaptomus salinus*, also from the copepod *Euchaeta russelli* and in aplanospores of *Haematococcus pluvialis* and fish skins.

Bartlett, L. *et al*, *J. Chem. Soc. C*, 1969, 2527 (*ord*)
Andrewes, A.G. *et al*, *Acta Chem. Scand.*, *Ser. B*, 1974, **28**, 730 (*synth*, *uv*)
Englert, G., *Helv. Chim. Acta*, 1975, **58**, 2367 (*cmr*)
Bandaranayake, W.M. *et al*, *Comp. Biochem. Physiol. B*: *Comp. Biochem.*, 1982, **72**, 409; *CA*, **98**, 14534n (*isol*)

Cubene C-80160

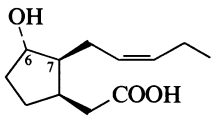
Pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]oct-1-ene, 9CI. 1,2-Dehydrocubane
[77478-10-5]

C_8H_6 M 102.135
Transient intermediate trapped by Diels Alder addn.

Eaton, P.E. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 7230 (*synth*)

Cucurbic acid C-80161

Updated Entry replacing C-50302
3-Hydroxy-2-(2-pentenyl)cyclopentaneacetic acid



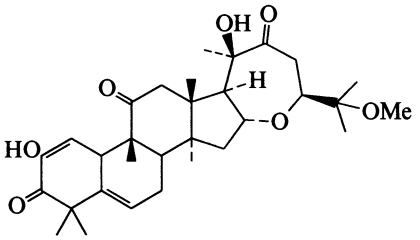
$C_{12}H_{20}O_3$ M 212.288
Constit. of *Cucurbita pepo*. Gum.

6,7-Diepimer: ***6-Epi-7-isocucurbic acid***
$C_{12}H_{20}O_3$ M 212.288
Constit. of *Vicia faba*. Oil. $[\alpha]_D^{22}$ +6.1° (c, 0.1 in EtOH).

Fukui, H. *et al*, *Agric. Biol. Chem.*, 1977, **41**, 175 (*isol*)
Kitahara, T. *et al*, *Agric. Biol. Chem.*, 1987, **51**, 1129 (*synth*)
Miersch, O. *et al*, *Phytochemistry*, 1989, **28**, 339 (*isol*)

Cucurbitacin T C-80162

[118172-78-4]

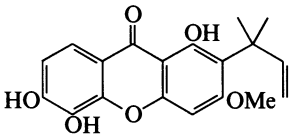


$C_{31}H_{44}O_7$ M 528.684
Constit. of *Colocynthis vulgaris*. Pale yellow semisolid. $[\alpha]_D^{28}$ −53.5° (c, 1.44 in $CHCl_3$).

Gamlath, C.B. *et al*, *Phytochemistry*, 1988, **27**, 3225.

Cudraniaxanthone C-80163

2-(1,1-Dimethyl-2-propenyl)-1,5,6-trihydroxy-3-methoxy-9H-xanthen-9-one, 9CI
[38710-42-8]

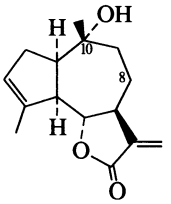


$C_{19}H_{18}O_6$ M 342.348
Constit. of the roots of *Cudrania javanensis*. Mp 308°.
Tri-Me ether: Mp 122-124°.

Murti, V.V.S. *et al*, *Phytochemistry*, 1972, **11**, 2089.

Cumambranolide C-80164

Updated Entry replacing C-40184
10α-Hydroxy-3,11(13)-guaiadien-12,6α-olide. 8-Deoxycumambrin B
[21956-65-0]



$C_{15}H_{20}O_3$ M 248.321
Constit. of *Artemisia nova* and *A. tripartita* ssp. *rupicola*. Prisms (Et_2O/pet. ether). Mp 117-118°.

8α-Hydroxy: [21982-83-2]. ***Cumambrin B***
$C_{15}H_{20}O_4$ M 264.321
Constit. of *A. nova*, *A. tripartita* ssp. *rupicola*, *Ambrosia cumanensis* and *A. acanthicarpa*. Cryst. (EtOAc/Et_2O). Mp 178-180°. $[\alpha]_D$ +92.5° (c, 5.58 in $CHCl_3$).

8α-Acetoxy: [20482-33-1]. ***Cumambrin A***
$C_{17}H_{22}O_5$ M 306.358
Constit. of *Artemesia nova*, *A. tripartita* ssp. *rupicola*, *Ambrosia cumanensis* and *A. acanthicarpa*. Cryst. Mp 188-190°. $[\alpha]_D$ +103° (c, 2.79 in $CHCl_3$).

8α-(2-Methylpropanoyloxy):
$C_{19}H_{26}O_5$ M 334.411
Constit. of *Eremanthus incanus*. Cryst. (Et_2O/pet. ether). Mp 130°. $[\alpha]_D^{24}$ +84.1° (c, 0.22 in $CHCl_3$).

8α-(2-Methylpropenoyloxy):
$C_{19}H_{24}O_5$ M 332.396
Constit. of *Lychnophora blanchetti*. Gum.

8α-Tigloyloxy:
$C_{20}H_{26}O_5$ M 346.422
Constit. of *L. blanchetti*. Gum.

8α-Angeloyloxy:
$C_{20}H_{26}O_5$ M 346.422
Constit. of *Chrysanthemum ornatum*. Antimicrobial. Oil. $[\alpha]_D^{20}$ +100° (c, 0.2 in MeOH).

8β-Hydroxy: Cryst. (MeOH). Mp 91-92°.

8β-Angeloyloxy:
$C_{20}H_{26}O_5$ M 346.422
Constit. of *Helianthus maximiliani*. Cryst. (EtOAc). Mp 160-161°.

8β-(Epoxyangeloyloxy):
$C_{20}H_{26}O_6$ M 362.422
From *H. maximiliani*. Oil.

8β-(3-Hydroxy-2-methylenebutanoyloxy):
$C_{20}H_{26}O_6$ M 362.422
From *H. maximiliani*. Oil.

8β-Sarracinoyloxy:
$C_{20}H_{26}O_6$ M 362.422
From *H. maximiliani*. Cryst. (diisopropyl ether/MeOH). Mp 129-130°.

8α-Acetoxy, 11β,13-Dihydro: ***Dihydrocumambrin A***
$C_{17}H_{24}O_5$ M 308.374
From *C. coronarium*. Cryst. Mp 174°. $[\alpha]_D^{24}$ +44° (c, 0.08 in $CHCl_3$).

10-O-β-D-Glucopyranoside: [100187-65-3]. ***Macrocliniside G***
$C_{21}H_{30}O_8$ M 410.463
Constit. of *Macroclinidium trilobum*. Needles (MeOH aq.). Mp 128-129°. $[\alpha]_D^{25}$ +39.8° (c, 1.86 in MeOH).

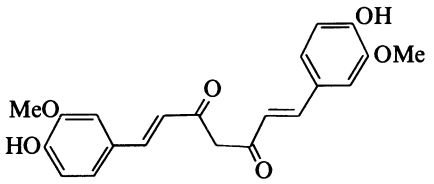
10-Epimer: ***10-Epicumambranolide.*** *10-Epi-8-deoxycumambrin B*
$C_{15}H_{20}O_3$ M 248.321
Constit. of *Stevia yaconensis*. Cryst. (Et_2O). Mp 123-124°.

Romo, J. *et al*, *Tetrahedron*, 1968, **24**, 5625 (*isol*)
Irwin, M.A. *et al*, *Phytochemistry*, 1969, **8**, 305 (*isol*)
Bohlmann, F.B. *et al*, *Phytochemistry*, 1980, **19**, 2663, 2669 (*isol*)
Haruna, M. *et al*, *Phytochemistry*, 1981, **20**, 2583 (*isol*)
Watson, W.H. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 1608 (*cryst struct*)
Gershenzon, J. *et al*, *Phytochemistry*, 1984, **23**, 1959 (*isol*)
El-Masry, S. *et al*, *Phytochemistry*, 1984, **23**, 2953 (*isol*)
Miyase, T. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 4445 (*isol*)
Sosa, V.E. *et al*, *Phytochemistry*, 1989, **28**, 1925 (*isol, cryst struct*)

Curcumin C-80165

Updated Entry replacing C-20253

1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, 9CI. Curcuma yellow. Diferuloylmethane
[458-37-7]



$C_{21}H_{20}O_6$ M 368.385
Isol. from *Curcuma* spp. (turmeric). Natural colouring matter used extensively in Indian curries etc. Orange prisms. Mp 183°.

Di-Ac: Cryst. Mp 170-171°.

Dibenzoyl: Cryst. Mp 210°.

Demethoxy: [22608-11-3]. *1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, 9CI.* p-Hydroxycinnamoylferuloylmethane. ***Demethoxycurcumin***
$C_{20}H_{18}O_5$ M 338.359
Isol. from *C. longa, C. domestica, C. xanthorrhiza*. Orange-yellow powder. Mp 168°.

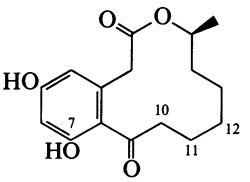
Bis-demethoxy: [22608-12-4]. *1,7-Bis(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, 9CI.* p,p′-*Dihydroxydicinammoylmethane.* ***Bisdemethoxycurcumin***
$C_{19}H_{16}O_4$ M 308.333
Isol. from *C. longa, C. domestica* and *C. aromatica*. Absent in some *C.* spp. Yellow plates + H_2O (EtOH). Mp 224°.

[24939-16-0, 33171-05-0]

Lampe, V., *Ber.*, 1918, **51**, 1347 (*synth*)
Srinivasan, K.R., *J. Pharm. Pharmacol.*, 1953, **5**, 448 (*derivs*)
Jentzsch, K. *et al*, *Sci. Pharm.*, 1968, **36**, 251; *CA*, **70**, 90793h (*isol*)
Sastry, B.S., *Res. Ind.*, 1970, **15**, 258; *CA*, **75**, 75063e (*isol*)
Kuroyagi, M. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1970, **90**, 1467; *CA*, **74**, 61612a (*isol*)
Roughley, P.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 2379 (*biosynth*)
Karig, F., *Dtsch. Apoth.-Ztg.*, 1975, **115**, 325; *ca*, **83**, 65372f (*derivs*)
Kashina, C. *et al*, *Heterocycles*, 1977, **7**, 241 (*synth*)
Wahlstrom, B. *et al*, *Acta Pharmacol. Toxicol.*, 1978, **43**, 86 (*metab*)
Holder, G.M. *et al*, *Xenobiotica*, 1978, **8**, 761 (*metab*)
Tønnesen, H.H. *et al*, *Acta Chem. Scand., Ser. B*, 1982, **36**, 475 (*cryst struct, bibl*)

Curvularin C-80166

Updated Entry replacing C-03021



$C_{16}H_{20}O_5$ M 292.331

(S)-form [10140-70-2]
Isol. from *Curvularia* spp., *Penicillium gilmanii, Alternaria cinerariae* and *A. macrospora*. Phytotoxin. Cryst. (MeOH/C_6H_6). Mp 206°. $[\alpha]_D^{18}$ −36.3°.

Di-Me ether: Cryst. (MeOH aq.). Mp 72°, Mp 105-108°. $[\alpha]_D^{18}$ −2.9° (c, 2.7 in $CHCl_3$).

Dibenzoyl: Cryst. (C_6H_6/pet. ether). Mp 133-134°. $[\alpha]_D^{18}$ −10.8° (c, 1.9 in $CHCl_3$).

10,11-Didehydro(E-): [21178-57-4]. **trans-*Dehydrocurvularin***
$C_{16}H_{16}O_5$ M 288.299
From *C.* spp., *A. cinerariae* and *A. macrospora*. Phytotoxin. Mp 224°. $[\alpha]_D^{22}$ −79.8° (c, 3.0 in EtOH).

10,11-Didehydro(E-), *7-Ac:*
$C_{18}H_{18}O_6$ M 330.337
From *C. scirpicola*. Mp 105-110°. $[\alpha]_D^{20}$ −31.7° (c, 0.4 in MeOH).

10,11-Didehydro(Z-): **cis-*Dehydrocurvularin***
$C_{16}H_{18}O_5$ M 290.315
Metabolite of hybrid strain of *Penicillium citreo-viride B*. Amorph. powder. $[\alpha]_D^{22}$ +7.3° (c, 0.78 in EtOH).

12-Oxo: ***12-Oxocurvularin***
$C_{16}H_{18}O_6$ M 306.315
Metabolite of *P. citreo-viride B*. Amorph. powder. $[\alpha]_D^{29}$ −43.5° (c, 0.47 in EtOH).

11α-Hydroxy: ***11α-Hydroxycurvularin***
$C_{16}H_{20}O_6$ M 308.330
Metabolite of *P. citreo-viride B*. Cryst. Mp 150-152°. $[\alpha]_D^{26}$ −29.4° (c, 0.33 in EtOH).

11β-Hydroxy: ***11β-Hydroxycurvularin***
$C_{16}H_{20}O_6$ M 308.330
Metabolite of *P. citreo-viride B.* Cryst. Mp 138-140°. $[\alpha]_D^{24}$ −10.9° (c, 0.19 in EtOH).
(±)-***form*** [65690-37-1]
Mp 182-184°.

Birch, A.J. *et al*, *J. Chem. Soc.*, 1959, 3146 (*isol*)
Baker, P.M. *et al*, *J. Chem. Soc. C*, 1967, 1913 (*synth*)
Munro, H.D. *et al*, *J. Chem. Soc. C*, 1967, 947 (*deriv*)
Coombe, R.G. *et al*, *Aust. J. Chem.*, 1968, **21**, 783 (*isol*)
Raistrick, H. *et al*, *J. Chem. Soc. C*, 1971, 3069 (*isol*)
Gerlach, H., *Helv. Chim. Acta*, 1977, **60**, 3039 (*synth*)
Assante, G. *et al*, *Phytochemistry*, 1977, **16**, 243 (*deriv*)
Takahashi, T. *et al*, *Tetrahedron Lett.*, 1980, **21**, 3885 (*synth*)
Robeson, D.J. *et al*, *Z. Naturforsch.*, *C*, 1981, **36**, 1081; *J. Nat. Prod.* (*Lloydia*), 1985, **48**, 139 (*isol*)
Lai, S., *Tetrahedron Lett.*, 1989, **30**, 2241 (*derivs*)

Cyanic acid C-80167

Updated Entry replacing C-03036
Hydrogen cyanate
[420-05-3]

HOC≡N

CHNO M 43.025
Is not in equilib. with Isocyanic acid, I-80057. Refs. are freq. confused in CA. Obt. in Ar matrix. Kinetically unstable.

Jacox, M.E. *et al*, *J. Chem. Phys.*, 1964, **40**, 2457.
Groving, N. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1768 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 170.
Bondybey, V.E. *et al*, *J. Mol. Spectrosc.*, 1982, **92**, 431 (*ir*, *uv*)
Teles, J.H. *et al*, *Chem. Ber.*, 1989, **122**, 753 (*struct*, *bibl*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 526.

N-Cyanobenzenecarboximidoyl chloride C-80168

[107129-18-0]

PhCCl=NCN

$C_8H_5ClN_2$ M 164.594
Solid. Mp 81°. $Bp_{0.2}$ 110°.

Hartke, K. *et al*, *Chem. Ber.*, 1989, **122**, 657 (*synth*, *pmr*, *cmr*)

Cyanogen fluoride, 9CI, 8CI C-80169

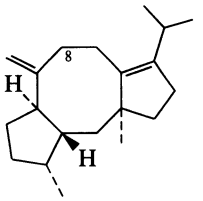
Updated Entry replacing C-20257
Fluoroformonitrile
[1495-50-7]

FCN

CFN M 45.016
Mp −72° subl.
▷ Can polymerise explosively.

Fawcett, F.S. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 1509 (*synth*, *props*)
Bieri, G., *Chem. Phys. Lett.*, 1977, **46**, 107 (*uv*)
Shimanoachi, T., *J. Phys. Chem. Ref. Data*, 1977, **6**, 993 (*ir*)
Bauknight, C.W. *et al*, *J. Org. Chem.*, 1988, **53**, 4443 (*synth*, *haz*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 283.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 528.

Cycloaraneosene C-80170



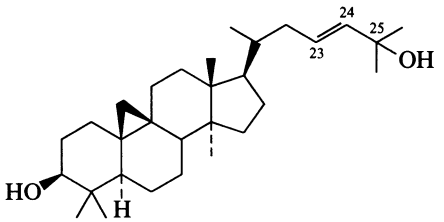
$C_{20}H_{32}$ M 272.473
Constit. of *Sordaria araneosa*. Oil. $[\alpha]_D^{27}$ −37.5° (c, 0.21 in $CHCl_3$).

8β-Hydroxy: ***8β-Hydroxycycloaraneosene***
$C_{20}H_{32}O$ M 288.472
Constit. of *S. araneosa*. Oil. $[\alpha]_D$ +15°.

Borschberg, H.J., *Ph.D. Thesis*, ETH, Zurich, 1975 (*isol*)
Kato, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3231 (*synth*)
Kato, N. *et al*, *Chem. Lett.*, 1989, 91 (*synth*)

23-Cycloartene-3,25-diol C-80171

9,19-Cyclolanost-23-ene-3,25-diol, 9CI



$C_{30}H_{50}O_2$ M 442.724
3β-form [14599-48-5]
Isol. from *Tillandsia usneoides* and *Tricholepsis glaberrima*. Prisms (EtOAc). Mp 200-204°. $[\alpha]_D^{27}$ +38° (c, 0.85 in $CHCl_3$).

3-Ac: [26531-71-5].
$C_{32}H_{52}O_3$ M 484.761
Isol. from roots of *Sapium insigne*. Prisms (hexane). Mp 148-150°. $[\alpha]_D^{22}$ +43° (c, 0.75 in $CHCl_3$).

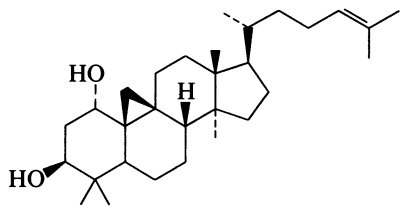
Di-Ac: Cryst. (Et_2O). Mp 105-108°.

O^{25}-*Me: 25-Methoxy-23-cycloarten-3β-ol*
$C_{31}H_{52}O_2$ M 456.751
Isol. from *Tillandsia usneoides*. Isol. as acetate.

O^{25}-*Me*,O^3-*Ac:* Needles ($MeOH/Et_2O$). Mp 152-154°. $[\alpha]_D^{28}$ +48° (c, 0.75 in $CHCl_3$).

Djerassi, C. *et al*, *J. Chem. Soc.*, 1962, 4034 (*isol*, *ir*, *pmr*, *struct*)
Fourrey, J.L. *et al*, *Tetrahedron*, 1970, **26**, 3839 (*synth*)
Chawla, A.S. *et al*, *Planta Med.*, 1978, **34**, 109 (*isol*)
Srivastava, S.K. *et al*, *J. Nat. Prod.* (*Lloydia*), 1985, **48**, 496 (*acetate*, *isol*, *pmr*)

24-Cycloartene-1,3-diol C-80172



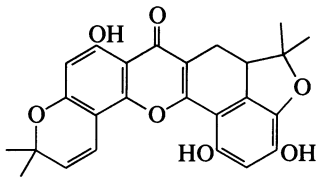
$C_{30}H_{50}O_2$ M 442.724
(1α,3β)-form
1-Ac: [119765-93-4]. *1α-Acetoxy-24-cycloarten-3β-ol*
$C_{32}H_{52}O_3$ M 484.761

Constit. of *Commiphora incisa*. Amorph. solid.

[119765-93-4]

Provan, G.J. *et al*, *Phytochemistry*, 1988, **27**, 3841.

Cycloartobiloxanthone C-80173



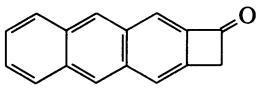
$C_{25}H_{22}O_7$ M 434.445

Constit. of *Artocarpus nobilis*. Dark yellow solid (MeOH). Mp 285-287°.

Sultanbawa, M.U.S. *et al*, *Phytochemistry*, 1989, **28**, 599.

Cyclobuta[*b*]anthracen-1(2*H*)one C-80174

1,2-Dihydrocyclobuta[b]*anthracen-1-one*



$C_{16}H_{10}O$ M 218.254

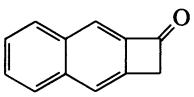
Yellow solid. Mp 230-251° dec.

Müller, P. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1618 (*synth*, *uv*, *ir*, *pmr*, *ms*)

Cyclobuta[*b*]naphthalen-1(2*H*)-one C-80175

Naphtho[b]*cyclobutenone*

[89185-31-9]



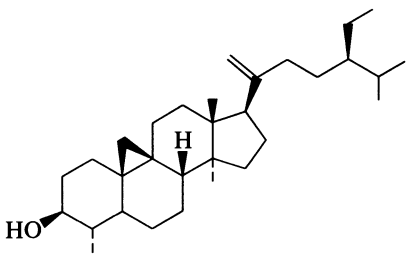
$C_{12}H_8O$ M 168.195

Cryst. (CCl_4). Mp 163-164°.

2,4-Dinitrophenylhydrazone: Orange cryst. (EtOAc). Mp 266-269°.

Abou-Teim, O. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1983, 2659 (*synth*, *uv*)

Cyclocaducinol C-80176

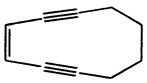


$C_{31}H_{52}O$ M 440.751

Constit. of *Euphorbia caducifolia*. Needles (Me_2CO). Mp 96-98°. $[\alpha]_D$ +48.9° (c, 0.16 in $CHCl_3$).

Afza, N. *et al*, *Phytochemistry*, 1989, **28**, 1982.

3-Cyclodecene-1,5-diyne, 9CI C-80177



$C_{10}H_{10}$ M 130.189

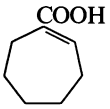
(Z)-form [115227-60-6]

Slowly dec. on standing.

Nicolaou, K.C. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4866 (*synth*, *pmr*, *cmr*, *uv*)

1-Cycloheptenecarboxylic acid C-80178

[4321-25-9]



$C_8H_{12}O_2$ M 140.182

Mp 54°. $Bp_{2.5}$ 124-125°.

Me ester:

$C_9H_{14}O_2$ M 154.208

Liq. $Bp_{0.15}$ 42-46°.

Et ester:

$C_{10}H_{14}O_2$ M 166.219

Bp_{22} 116-119°.

Amide:

$C_8H_{13}NO$ M 139.197

Needles (MeOH/EtOH). Mp 125-127°.

Nitrile: [20343-19-5]. *1-Cyanocycloheptene*

$C_8H_{11}N$ M 121.182

Liq. Bp_{12} 95-96°, $Bp_{0.25}$ 47-51°.

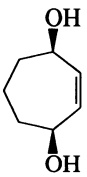
Ayerst, G.G. *et al*, *J. Chem. Soc.*, 1960, 3445 (*nitrile*, *amide*, *Et ester*, *synth*)

Braidy, R., *Bull. Soc. Chim. Fr.*, 1967, 3489 (*synth*, *ir*, *cryst struct*)

Mathur, K.C. *et al*, *Indian J. Chem.*, 1968, **6**, 248 (*synth*, *nitrile*, *Et ester*)

Pawlak, J.L. *et al*, *J. Org. Chem.*, 1988, **53**, 4063 (*nitrile*, *Me ester*, *synth*, *pmr*)

2-Cycloheptene-1,4-diol C-80179



$C_7H_{12}O_2$ M 128.171

(1RS,4SR)-form

cis-form

Di-Me ether: [116910-22-6]. *2,7-Dimethoxycycloheptene*

$C_9H_{16}O_2$ M 156.224

Oil. Bp_2 130° (kugelrohr) .

Di-Et ether: [90786-03-1]. *2,7-Diethoxycycloheptene*

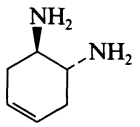
$C_{11}H_{20}O_2$ M 184.278

Oil. Bp_2 140° (kugelrohr) .

Bäckvall, J.E. *et al*, *J. Org. Chem.*, 1988, **53**, 5695 (*synth*, *pmr*, *cmr*, *ir*)

4-Cyclohexene-1,2-diamine, 9CI C-80180

4,5-Diaminocyclohexene



(1*RS*,2*RS*)-*form*

$C_6H_{12}N_2$ M 112.174

(1RS,2RS)-form

(±)trans-form

B,2HCl: [108796-57-2].
Powder. Mp >280°.

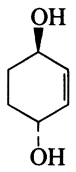
(1RS,2SR)-form

cis-form

B,2HCl: [105249-35-2].
Powder. Mp 255-256°.

Witiak, D.T. *et al*, *J. Med. Chem.*, 1987, **30**, 1327 (*synth, pmr, ir*)

2-Cyclohexene-1,4-diol, 9CI C-80181



(1*RS*,4*RS*)-*form*

$C_6H_{10}O_2$ M 114.144

(1RS,4RS)-form [41513-32-0]

(±)-*trans form*
Cryst. Mp 83-84°.

Di-Ac: [78776-44-0].
Cryst. (hexane). Mp 49-50°.

(1RS,4SR)-form [53762-85-9]

cis-form
Cryst. Mp 57-59°.

Di-Ac: [78776-45-1].
$C_{10}H_{14}O_4$ M 198.218
Liq.

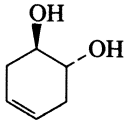
Di-Me ether: [59415-77-9]. *3,6-Dimethoxycyclohexene*
$C_8H_{14}O_2$ M 142.197
Oil. Bp_2 120°.

Di-Et ether: [90786-01-9]. *3,6-Diethoxycyclohexene*
$C_{10}H_{18}O_2$ M 170.251
Oil. Bp_1 75° (kugelrohr) .

Dibenzyl ether: [116910-21-5].
$C_{20}H_{22}O_2$ M 294.393
Oil. $Bp_{0.3}$ 230°.

Kaneko, C. *et al*, *Synthesis*, 1974, 876 (*synth, pmr*)
Bäckvall, J.-E. *et al*, *J. Org. Chem.*, 1984, **49**, 4619; 1988, **53**, 5695 (*synth, pmr, cmr, ir*)

4-Cyclohexene-1,2-diol C-80182



(1*R*,2*R*)-*form*

$C_6H_{10}O_2$ M 114.144

(1R,2R)-form

Mono-Ac:
$C_8H_{12}O_3$ M 156.181
Mp 71°. $[\alpha]_D^{22}$ −121.6° (c, 0.86 in $CHCl_3$).

(1RS,2RS)-form

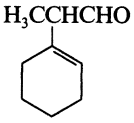
(±)-trans-*form*
Needles (EtOAc/hexane). Mp 95°.

Di-Ac:
$C_{10}H_{14}O_4$ M 198.218
Oil.

Suemune, H. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1379.

2-(1-Cyclohexenyl)propanal C-80183

α-Methyl-1-cyclohexene-1-acetaldehyde, 9CI



$C_9H_{14}O$ M 138.209

(±)-***form*** [114221-81-7]

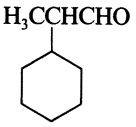
Oil.

Tsukamoto, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 880 (*synth*)
Maruoka, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3588 (*synth, pmr, ir*)

2-Cyclohexylpropanal C-80184

α-Methylcyclohexaneacetaldehyde, 9CI

[2109-22-0]



$C_9H_{16}O$ M 140.225

(±)-***form*** [97859-57-9]

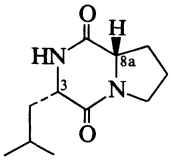
Oil.

Meyers, A.I. *et al*, *Tetrahedron*, 1985, **41**, 5089 (*synth, pmr, ir*)
Maruoka, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3588 (*synth, pmr*)

Cyclo(leucylprolyl) C-80185

Hexahydro-3-(2-methylpropyl)pyrrolo[1,2a]pyrazine-1,4-dione. Gancidin W

[5654-86-4]



$C_{11}H_{18}N_2O_2$ M 210.275
Diketopiperazine antibiotic.

(3S,8aS)-form [2873-36-1]

L,L-*form*
Prod. by *Streptomyces gancidicus, Nocardia restricta, Candida albicans, Guignardia laricina* and several *Ceratocystis* spp. Also isol. from the sponge *Tedania ignis*. Bitter component of sake and contributes to the flavour of beer. Shows antitumour and antifungal props. Phytotoxin associated with fungal diseases of trees.
Cryst. Mp 168-172° (158-159°). $[\alpha]_D^{25-28}$ −133° (c, 1 in EtOH), $[\alpha]_D^{21}$ −144° (c, 0.5 in H_2O).

▷ UY8708800.

(3R,8aS)-form [36238-67-2]

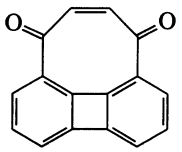
Cryst. Mp 148-149° (119-122°). $[\alpha]_D^{31}$ −105.5° (c, 0.5 in EtOH).

[19943-30-7, 43041-29-8]

Kodaira, Y. *et al*, *Agric. Biol. Chem.*, 1961, **25**, 261.
Nitecki, D.E. *et al*, *J. Org. Chem.*, 1968, **33**, 864 (*synth*)
Siemion, I.Z. *et al*, *Org. Magn. Reson.*, 1971, **3**, 545 (*synth, nmr*)
Vicar, J. *et al*, *Collect. Czech. Chem. Commun.*, 1972, **37**, 4060; 1973, **38**, 1940 (*synth, ir, pmr*)
Karle, I.L., *J. Am. Chem. Soc.*, 1972, **94**, 81 (*cryst struct*)
Takahashi, K. *et al*, *Agric. Biol. Chem.*, 1974, **38**, 927.
Bycroft, B.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 988 (*synth*)
Davies, D.B. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1976, 187 (*conformn*)
Pancoska, P. *et al*, *Collect. Czech. Chem. Commun.*, 1977, **44**, 1296 (*cd*)
Jain, T.C. *et al*, *Heterocycles*, 1977, **7**, 341 (*isol, struct, uv, ms*)
Bjoerkman, S. *et al*, *J. Med. Chem.*, 1979, **22**, 931 (*synth*)
Suzuki, K. *et al*, *Chem. Pharm. Bull.*, 1981, **29**, 233 (*synth*)
Schmidtz, F.J. *et al*, *J. Org. Chem.*, 1983, **48**, 3941 (*isol, ms, pmr, synth, bibl*)
Ayer, W.A. *et al*, *Can. J. Chem.*, 1986, **64**, 904 (*isol*)
Kricheldorf, H.R. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 21 (*cmr*)

Cycloocta[*def*]biphenylene-1,4-dione C-80186

[119392-56-2]

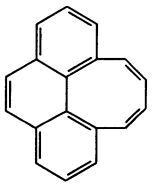


$C_{16}H_8O_2$ M 232.238
Yellow solid. Mp 162-165°. Non-planar structure.

Wilcox, C.F. *et al*, *J. Org. Chem.*, 1989, **54**, 2190 (*synth, pmr, cmr, ms, cryst struct*)

Cycloocta[*def*]phenanthrene C-80187

[111409-91-7]



$C_{18}H_{12}$ M 228.293

Heinz, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 1291 (*synth, pmr, cmr, uv*)

1,3,5-Cyclooctatriene, 9CI C-80188

Updated Entry replacing C-03516

[1871-52-9]

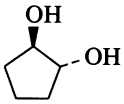
C_8H_{10} M 106.167
Liq. d_4^{25} 0.897. Bp 145-146°, Bp_{90} 76°.
$AgNO_3$ complex: Cryst. (EtOH). Mp 125-126°.

Cope, A.C. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 4867 (*synth*)
Tarakanova, A.V. *et al*, *Zh. Org. Khim.*, 1972, **8**, 1619 (*synth*)
Anet, F.A.L. *et al*, *Tetrahedron Lett.*, 1975, 4221 (*conformn*)
Bally, T. *et al*, *Helv. Chim. Acta*, 1989, **72**, 73 (*synth, bibl*)

1,2-Cyclopentanediol, 9CI C-80189

Updated Entry replacing C-03608

[4065-92-3]



(1*R*,2*R*)-*form*

$C_5H_{10}O_2$ M 102.133

(1R,2R)-form [63261-45-0]
(−)-trans-*form*
Mp 48-48.5°. $[\alpha]_D^{20}$ −24.88° (c, 6.0 in EtOH).
Phenylurethane: Mp 213-215°.

(1S,2S)-form [107492-82-0]
Fragrant solid. Mp 47.0-48.0°. $[\alpha]_D^{20}$ +24.54° (c, 5.4 in EtOH). Highly hygroscopic.

(1RS,2RS)-form [5057-99-8]
(±)-trans-*form*
Mp 55°. Bp_{22} 136°.
Di-Ac: [65783-98-4].
$C_9H_{14}O_4$ M 186.207
Mp −4°. $Bp_{3.5}$ 86°.
Dibenzoyl:
$C_{19}H_{18}O_4$ M 310.349
Mp 63°.
Bis(4-methylbenzenesulfonyl): Mp 109°.

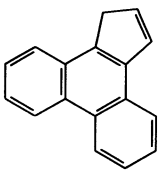
(1RS,2SR)-form [5057-98-7]
cis-*form*
Mp 30°. Bp_{29} 123.5°.
Di-Ac: [37854-32-3].
Mp −5°. Bp_2 80°.
Dibenzoyl: [37854-33-4].
Mp 47°.

[86703-52-8]

Verkade, P.E., *Justus Liebigs Ann. Chem.*, 1930, **477**, 279, 289 (*synth*)
Owen, L.N. *et al*, *J. Chem. Soc.*, 1952, 4026 (*synth*)
Singy, G.A. *et al*, *Helv. Chim. Acta*, 1971, **54**, 537 (*ms*)
Kono, H. *et al*, *Org. Prep. Proced. Int.*, 1974, **6**, 19 (*synth*)
Mangoni, L. *et al*, *Gazz. Chim. Ital.*, 1975, **105**, 377 (*synth*)
Cunningham, A.F. *et al*, *J. Org. Chem.*, 1988, **53**, 1823 (*synth, ir, pmr*)

1*H*-Cyclopenta[*l*]phenanthrene, 9CI C-80190

[235-92-7]



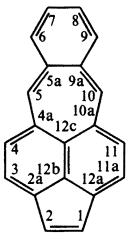
$C_{17}H_{12}$ M 216.282
Cryst. (2-propanol). Mp 150-152°.

Cope, A.C. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 2547 (*synth*)

Cyclopenta[*cd*]pleiadene, 9CI C-80191

Benz[h]*acepleiadylene. Acepleiadylene*

[193-60-2]



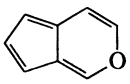
$C_{20}H_{12}$ M 252.315

Diels-Alder diene. Obt. as a deep blue soln., could not be isol. but dec. to polymeric material and a dimer.

Cava, M.P. *et al*, *Tetrahedron*, 1965, **21**, 3051, 3059, 3073 (*synth, uv, props*)

Cyclopenta[*c*]pyran C-80192

[270-61-1]



C_8H_6O M 118.135

Unstable oil.

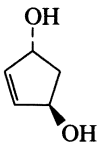
Kämpchen, T. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 855 (*synth, uv, pmr, cmr*)

4-Cyclopentene-1,3-diol, 9CI C-80193

Updated Entry replacing C-50374

3,5-Dihydroxycyclopentene

[4157-01-1]



(1*R*,3*R*)-*form*

$C_5H_8O_2$ M 100.117

(1R,3R)-form

Di-Ac: [60410-14-2].

$C_9H_{12}O_4$ M 184.191

$[\alpha]_D^{20}$ +208° (c, 0.025 in MeOH).

(1RS,3RS)-form [694-47-3]

(±)-trans-*form*

$Bp_{0.5}$ 100-105°. n_D^{25} 1.5024. V. hygroscopic.

Dibenzoyl:

$C_{19}H_{16}O_4$ M 308.333

Mp 124°.

Bis(3,5-dinitrobenzoyl): Mp 218-219°.

(1RS,3SR)-form [29783-26-4]

cis-*form*

Cryst. (EtOAc/pet. ether). Mp 59-61°. An achiral diol having synthetically important chiral monoacyl etc. blocked derivs.

Mono-Ac:

$C_9H_{12}O_4$ M 184.191

Cryst (Et_2O/pentane). Mp 47.5-48°. $[\alpha]_D^{22}$ +75.0° (c, 1.16 in $CHCl_3$).

Dibenzoyl: Mp 58-60°.

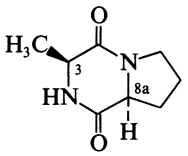
Bis(3,5-dinitrobenzoyl): Mp 208-209°.

[54664-61-8, 59415-74-6, 60389-71-1, 61826-75-3]

Sable, H.Z. *et al*, *Helv. Chim. Acta*, 1962, **41**, 371; 1963, **46**, 1157 (*synth, bibl*)
Cocu, F.G. *et al*, *Helv. Chim. Acta*, 1970, **53**, 739 (*pmr*)
Singy, G.A. *et al*, *Helv. Chim. Acta*, 1973, **56**, 449 (*ms*)
Org. Synth., Coll. Vol., 5, 1973, 416 (*synth*)
Kaneko, C. *et al*, *Synthesis*, 1974, 876 (*synth*)
Muira, S. *et al*, *Tetrahedron*, 1976, **32**, 1893 (*synth*)
Laumen, K. *et al*, *Tetrahedron Lett.*, 1984, **25**, 5875; 1985, **26**, 407 (*synth*)
Duhamel, L. *et al*, *Tetrahedron Lett.*, 1985, **26**, 3099 (*chiral deriv*)
Laumen, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 1298 (*derivs*)
Sugai, T. *et al*, *Synthesis*, 1988, 19 (*synth, pmr*)
Theil, F. *et al*, *Synthesis*, 1988, 540 (*synth, pmr*)

Cyclo(prolylalanyl) C-80194

*Hexahydro-3-methylpyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI*



(3*S*,8a*S*)-*form*

$C_8H_{12}N_2O_2$ M 168.195

(3S,8aS)-form [36357-32-1]

L,L-*form*. (3S-trans)-*form*

Isol. from cocoa; metab. product of the Caribbean sponge *Tedania ignis*. Mp 153-156°. $[\alpha]_{546}^{20}$ −160.0° (c, 1 in EtOH).

(3S,8aR)-form [19943-29-4]

D,L-*form*. (3S-cis-*form*)

From *Beauveria bassiana*. Mp 162-166°. $[\alpha]_D^{22}$ −85°.

(3R,8aS)-form [36238-64-9]

L,D-*form*. (3*R*-cis)-*form*

Mp 139-142°.

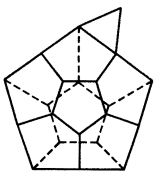
[19943-28-3, 65556-33-4]

Westley, J.W. *et al*, *Anal. Chem.*, 1968, **40**, 1888 (*glc, chromatog, pmr*)
Siemion, I.Z., *Org. Magn. Reson.*, 1971, **3**, 545 (*synth, pmr*)
Young, P.E. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 5365 (*synth, pmr, cmr*)
Izumiya, N. *et al*, *Pept. Chem.*, 1977, **15**, 49 (*pharmacol*)
Cotrait, M. *et al*, *Cryst. Struct. Commun.*, 1979, **8**, 819 (*cryst struct*)
Grove, J.F. *et al*, *Phytochemistry*, 1981, **20**, 815 (*isol*)
Schmitz, F.J. *et al*, *J. Org. Chem.*, 1983, **48**, 3941 (*isol, pmr, ms*)
Langhammer, M. *et al*, *Fresenius' Z. Anal. Chem.*, 1986, **324**, 5 (*ms*)

Cyclopropadodecahedrane C-80195

*Tetradecahydro-4*a*,2,1,5,3,3*c*-[2,3]butanediyl[1,4]diylidene-4*H*-cyclopropa[4,5]pentaleno[2,1,6-*cde*]pentaleno[2,1,6-*gha*]pentalene, 9CI*

[112896-42-1]



$C_{21}H_{20}$ M 272.389

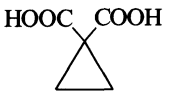
Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1305 (*synth*)

1,1-Cyclopropanedicarboxylic acid, 9CI C-80196

Updated Entry replacing C-03707

Ethylenemalonic acid. Vinaconic acid

[598-10-7]



$C_5H_6O_4$ M 130.100

Prisms or needles ($CHCl_3$), prisms + $1H_2O$ (H_2O). Sol. H_2O, org. solvs. Mp 140°. pK_{a1} 7.70 (7.67), pK_{a2} 2.92.

Di-Me ester: [6914-71-2].
$C_7H_{10}O_4$ M 158.154
Bp_{764} 198°.

Di-Et ester: [1559-02-0].
$C_9H_{14}O_4$ M 186.207
Liq. Bp_{22} 115°.

Mononitrile: [6914-79-0]. *1-Cyanocyclopropanecarboxylic acid*
$C_5H_5NO_2$ M 111.100
Mp 149° (140°).

Nitrile, Me ester: [6914-73-4]. *Methyl 1-cyanocyclopropanecarboxylate*
$C_6H_7NO_2$ M 125.127
Liq. Bp_{18} 92°.

Nitrile, Et ester: [1558-81-2]. *Ethyl 1-cyanocyclopropanecarboxylate*
$C_7H_9NO_2$ M 139.154
Bp 210-211°, Bp_{80} 137°.

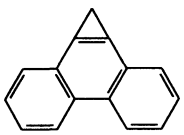
Nitrile, amide:
$C_5H_6N_2O$ M 110.115
Mp 160°.

Dinitrile: [1559-03-1]. *1,1-Dicyanocyclopropane*
$C_5H_4N_2$ M 92.100
Bp_{20} 103°. n_D^{25} 1.4463.

Perkin, W.H., *J. Chem. Soc.*, 1885, **47**, 807, 817.
Stewart, J.M. *et al*, *J. Org. Chem.*, 1965, **30**, 1951 (*dinitrile*)
Meester, M.A.M. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 630 (*cryst struct*)
Danishefsky, S. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 3239 (*synth*)
Jones, P.G. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 1576 (*cryst struct, mononitrile*)
Heiszman, J. *et al*, *Synthesis*, 1987, 738 (*deriv, synth, bibl*)

1*H*-Cyclopropa[*l*]phenanthrene C-80197

[278-91-1]

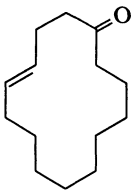


$C_{15}H_{10}$ M 190.244

Generated and trapped as adducts.

Dent, B.R. *et al*, *Aust. J. Chem.*, 1987, **40**, 925.

4-Cyclotetradecen-1-one, 9CI C-80198



$C_{14}H_{24}O$ M 208.343

[101999-70-6]

Porter, N.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3554 (*synth, ir, pmr, cmr*)

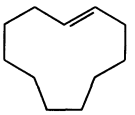
5-Cyclotetradecen-1-one C-80199

$C_{14}H_{24}O$ M 208.343

[75426-30-1, 114157-30-1]

Porter, N.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3554 (*synth, ir, pmr, cmr*)

Cycloundecene C-80200



(*E*)-*form*

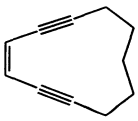
$C_{11}H_{20}$ M 152.279

(E)-form [13151-60-5]
Oil. Bp_{12} 88-90°, $Bp_{0.01}$ 25-30°.

(Z)-form [13151-61-6]
Bp_{12} 100°, $Bp_{0.01}$ 25-30°.

Fawcett, R.W. *et al*, *J. Chem. Soc.*, 1954, 2673 (*synth, uv*)
Prelog, V. *et al*, *Helv. Chim. Acta*, 1955, **38**, 1776 (*synth*)
Vilsmaier, E. *et al*, *J. Org. Chem.*, 1988, **53**, 1806 (*synth, ir, pmr*)

3-Cycloundecene-1,5-diyne, 9CI C-80201

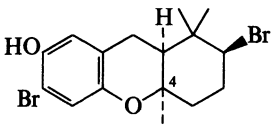


$C_{11}H_{12}$ M 144.216

(Z)-form [115227-61-7]
Large plates (pentane). Mp 36-36.5°.

Nicolaou, K.C. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4866 (*synth, cryst struct*)

Cymobarbatol C-80202



$C_{16}H_{20}Br_2O_2$ M 404.141

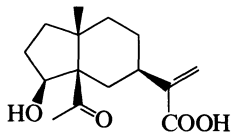
Metab. of *Cymopolia barbata*. Cryst. Mp 166°. $[\alpha]_D^{23}$ −15.4°.

4-Epimer: ***4-Isocymobarbatol***
$C_{16}H_{20}Br_2O_2$ M 404.141
Metab. of *C. barbata*. Cryst. Mp 147°. $[\alpha]_D^{23}$ −51.4°.

Wall, M.E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1092 (*pmr, cmr, cryst struct*)

Cyperanic acid C-80203

[117869-89-3]



$C_{15}H_{22}O_4$ M 266.336

Constit. of *Dittrichia viscosa*. Oil. $[\alpha]_D$ +26.3° (c, 0.004 in $CHCl_3$).

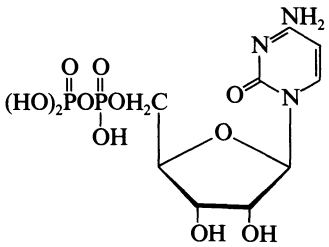
Me ester: Cryst. (Et_2O). Mp 62-64°.

Ceccherelli, P. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1006 (*isol, pmr, cmr*)

Cytidine-5′-diphosphate C-80204

Cytidine 5′-(trihydrogen diphosphate), 9CI. Cytidine pyrophosphate

[63-38-7]



$C_9H_{15}N_3O_{11}P_2$ M 403.178

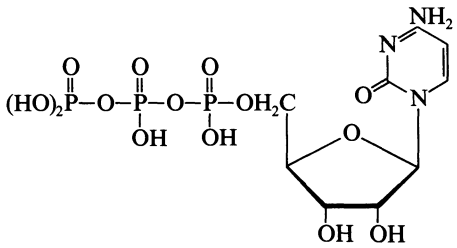
Exists as zwitterion. Prod. by *Plasmodium berghei* and *Bacillus brevis*. Found in heart, liver, leukaemia cells. Affects bladder contraction. Powder.

Kimura, A. *et al*, *Agric. Biol. Chem.*, 1975, **39**, 1469 (*manuf*)
Viswamitra, M.A. *et al*, *Nature* (*London*), 1975, **258**, 497 (*cryst struct*)
Labotka, R.J. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 3699 (*nmr*)
Iio, M. *et al*, *Agric. Biol. Chem.*, 1977, **41**, 155 (*synth*)
Kim, C.H. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 1571 (*conformn*)
Scheller, K.H. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 5891 (*pmr*)
Veda, T. *et al*, *J. Chromatogr.*, 1987, **386**, 273 (*hplc*)
Davisson, V.J. *et al*, *J. Org. Chem.*, 1987, **52**, 1794 (*synth, cmr, nmr, pmr*)

Cytidine 5′-triphosphate C-80205

Cytidine 5′-(tetrahydrogen triphosphate), 9CI

[65-47-4]



$C_9H_{16}N_3O_{14}P_3$ M 483.158

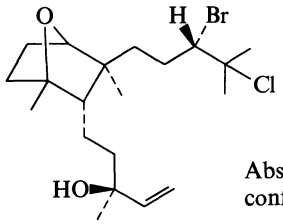
Prod. by *Leishmania* and *Streptomyces griseus*; found in cheese, brain, liver, erythrocytes and lymphocytes. Enzyme inhibitor. Implicated in purine and pyrimidine metabolism disorders. Contracts arteries.

Na salt: Cryst. powder.

Tanaka, K. *et al*, *Chem. Pharm. Bull.*, 1962, **10**, 220 (*synth*)
Lee, G.C.Y. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 951 (*tautom, pmr*)
Labotka, R.J. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 3699 (*nmr*)
Iio, M. *et al*, *Agric. Biol. Chem.*, 1977, **41**, 155 (*synth*)
Jost, W. *et al*, *Anal. Biochem.*, 1983, **135**, 120 (*chromatog*)
Kehr, J. *et al*, *Fresenius' Z. Anal. Chem.*, 1986, **325**, 466 (*hplc*)
Veda, T. *et al*, *J. Chromatogr.*, 1987, **386**, 273 (*hplc*)
Hammer, D.F. *et al*, *Anal. Biochem.*, 1988, **169**, 300 (*hplc*)

D

Dactylomelol **D-80001**

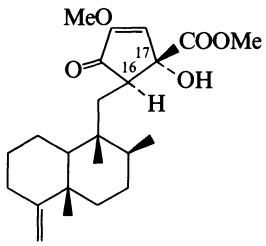


Absolute configuration

$C_{20}H_{34}BrClO_2$ M 421.844
Metab. of *Aplysia dactylomela*. Cryst. (CH_2Cl_2/hexane). Mp 85-86°. $[\alpha]_D^{20}$ −31.3° (c, 0.7 in $CHCl_3$).

Estrada, D.M. *et al*, *Tetrahedron Lett.*, 1989, **30**, 6219 (*cryst struct*)

Dactylospongenone A **D-80002**



$C_{23}H_{34}O_5$ M 390.519
Metab. of *Dactylospongia* sp. Cryst. $[\alpha]_D$ −167.7° (c, 0.062 in MeOH).

16-Epimer: ***Dactylospongenone D***
$C_{23}H_{34}O_5$ M 390.519
Metab. of *D.* sp. $[\alpha]_D$ −121.7° (c, 0.14 in MeOH).

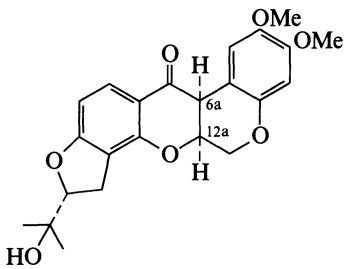
17-Epimer: ***Dactylospongenone C***
$C_{23}H_{34}O_5$ M 390.519
Metab. of *D.* sp. $[\alpha]_D$ +25.5° (c, 0.20 in MeOH).

16,17-Diepimer: ***Dactylospongenone B***
$C_{23}H_{34}O_5$ M 390.519
Metab. of *D.* sp. $[\alpha]_D$ +96.4° (c, 0.22 in MeOH).

Kushlan, D.M. *et al*, *Tetrahedron*, 1989, **45**, 3307 (*cryst struct*)

Dalpanol **D-80003**

Updated Entry replacing D-00015
6′,7′-Dihydro-6′-hydroxyrotenone



$C_{23}H_{24}O_7$ M 412.438
CA numbering shown. Isol. from ripe seeds of *Dalbergia paniculata*. Also from *Amorpha fruticosa*. Cryst. (C_6H_6). Mp 196°. $[\alpha]_D^{22}$ −136.3° ($CHCl_3$).

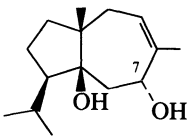
O-*Glucoside:*
$C_{29}H_{34}O_{12}$ M 574.580
Isol. from *D. paniculata* seeds. Cryst. solid. $[\alpha]_D^{34}$ −215.4° (c, 0.26 in 80% MeOH aq.).

6a,12a-Didehydro: ***Dehydrodalpanol***
$C_{23}H_{22}O_7$ M 410.423
Isol. from seeds of *D. paniculata*. Minute yellow needles ($CHCl_3$/MeOH). Mp 238-240°.

Adinarayana, D. *et al*, *J. Chem. Soc. C*, 1971, 29 (*isol*)
Crombie, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 1277 (*synth*)
Radhakrishniah, M. *et al*, *Phytochemistry*, 1973, **12**, 3003 (*glucoside*)
Adinarayana, D. *et al*, *Indian J. Chem.*, 1975, **13**, 425 (*Dehydrodalpanol*)
Crombie, L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 1143 (*biosynth*)

8-Daucene-5,7-diol **D-80004**

Carotdiol



$C_{15}H_{26}O_2$ M 238.369
Cryst. Mp 76-78°.

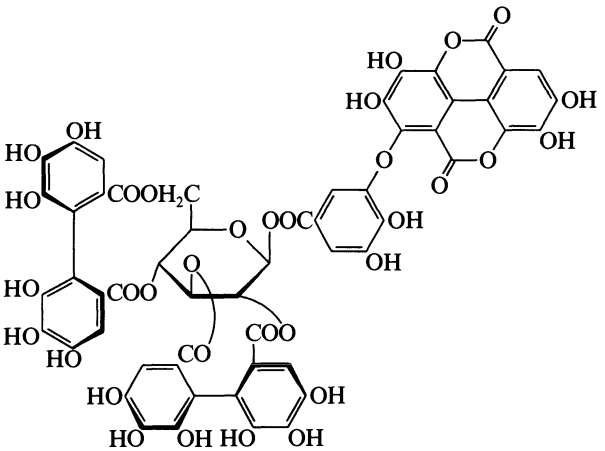
7-Ac: ***Carotdiol acetate***
$C_{17}H_{28}O_3$ M 280.406
Constit. of *Ferula linkii*. Oil.

7-(3,4-Dimethoxybenzoyl): ***Carotdiol veratrate***
$C_{24}H_{34}O_5$ M 402.530
Constit. of *F. linkii*. Oil.

Fraga, B.M. *et al*, *Phytochemistry*, 1989, **28**, 1649.

Daviciin M_1 **D-80005**

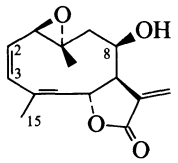
[119139-62-7]



$C_{55}H_{32}O_{34}$ M 1236.837
Constit. of *Rosa davurica*. Amorph. powder. $[\alpha]_D$ −58° (c, 1 in MeOH).

Yoshida, T. *et al*, *Phytochemistry*, 1989, **28**, 2177 (*isol, pmr, cmr*)

8-Deacyl-15-deoxypunctatin D-80006



$C_{15}H_{18}O_4$ M 262.305

8-O-(2-Methyl-2,3-epoxybutanoyl):
$C_{20}H_{24}O_6$ M 360.406
Constit. of *Trichogonia santosii*. Cryst. (Et_2O). Mp 173°. $[\alpha]_D^{24}$ −422° (c, 0.09 in $CHCl_3$).

2α,2α-Epoxy, 8-O-angeloyl: ***15-Deoxyliscundin***
$C_{20}H_{24}O_6$ M 360.406
Constit. of *T. santosii*. Oil.

2α,3α-Epoxy, 8-O-(2-methyl-2,3-epoxybutanoyl):
$C_{20}H_{24}O_7$ M 376.405
Constit. of *T. santosii*. Cryst. (Et_2O). Mp 198°. $[\alpha]_D$ −104° (C, 0.65 in $CHCl_3$).

2α,3α-Epoxy, 8-O-(2-hydroxymethyl-2Z-butenoyl):
$C_{20}H_{24}O_7$ M 376.405
Constit. of *T. santosii*. Cryst. (Et_2O). Mp 172°. $[\alpha]_D$ −135° (c, 0.2 in $CHCl_3$).

15-Hydroxy, 8-O-(2-hydroxymethyl-2Z-butenoyl): [49776-54-7]. ***Punctaliatrin.*** *Punctatin*
$C_{20}H_{24}O_7$ M 376.405
Constit. of *Liatris punctata*. Cryst. Mp 163-165°.

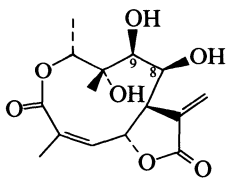
15-Hydroxy, 2α,3α-epoxy, 8-O-angeloyl: [57498-86-9]. ***Liscundin***
$C_{20}H_{24}O_7$ M 376.405
Constit. of *L. secunda*. Oil. $[\alpha]_D^{22}$ −75° (c, 2 in $CHCl_3$).

15-Hydroxy, 2α,3α-epoxy, 8-O-(2-acetoxymethyl-2Z-butenoyl): [57498-88-1]. ***Liscunditrin***
$C_{22}H_{26}O_9$ M 434.442
Constit. of *L. secunda*. Amorph. solid. Mp 161°. $[\alpha]_D^{22}$ −5° ($CHCl_3$).

Herz, W. *et al*, *Phytochemistry*, 1973, **12**, 1421 (*Punctaliatrin*)
Herz, W. *et al*, *Phytochemistry*, 1975, **14**, 1561 (*Liscundin, Liscunditrin*)
Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1984, 162 (*isol*)

8-Deacyltrichogoniolide D-80007

Updated Entry replacing T-02890



$C_{15}H_{20}O_7$ M 312.319

8-O-Angeloyl:
$C_{20}H_{26}O_8$ M 394.421
Constit. of *Trichogonia villosa*. Oil.

8-O-Angeloyl, 9-Ac:
$C_{22}H_{28}O_9$ M 436.458
Constit. of *T. histifolia*. Oil.

8-O-(2-Methylpropenoyl): [79694-65-8]. ***Trichogoniolide***
$C_{19}H_{24}O_8$ M 380.394
Constit. of *T. prancii*. Gum.

8-O-(2-Methylpropenoyl), 9-Ac:
$C_{21}H_{26}O_9$ M 422.431
Constit. of *T. prancii*. Cryst. (Et_2O). Mp 215°. $[\alpha]_D^{24}$ −246° (c, 0.7 in $CHCl_3$).

Bohlmann, F. *et al*, *Phytochemistry*, 1981, **20**, 1323 (*isol*)
Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1984, 162 (*isol*)

2,8-Decadiene-4,6-diyn-1-al, 9CI D-80008

Matricarianal

[30377-44-7]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCHO$

$C_{10}H_8O$ M 144.173
Isol. from underground parts of *Pimpinella magna*.

(E,E)-form [59950-66-2]
Isol. from above-ground parts of *Aethusa cynapium*. Yellowish cryst. (pet. ether). Mp 68.5°.

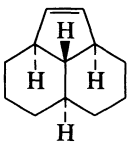
(2E,8Z)-form [13894-66-1]
$Bp_{0.1}$ 60-70°.

(2Z,8E)-form [29576-73-6]
Isol. from *Grindelia* sp.

Bohlmann, F. *et al*, *Chem. Ber.*, 1955, **88**, 1330; 1964, **97**, 2598; 1966, **99**, 3194; 1970, **103**, 2245 (*isol, uv, ir, pmr, synth*)
Schulte, K.E. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1970, **303**, 912 (*isol, uv, ir*)

2*a*,3,4,5,5*a*,6,7,8,8*a*,8*b*-Decahydroacenaphthene D-80009

Tricyclo[7.2.1.0^{5,12}]dodec-10-ene

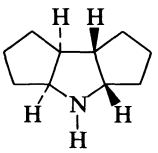


$C_{12}H_{18}$ M 162.274

(2aα,5aα,9aα,9bβ)-form [115650-98-1]
Ufolene
Bp_{20} 102°.

Boldt, P. *et al*, *Chem. Ber.*, 1980, **121**, 2029 (*synth, ir, pmr, cmr, ms*)

Decahydro-1*H*-dicyclopenta[*b,d*]pyrrole, 9CI D-80010



$C_{10}H_{17}N$ M 151.251

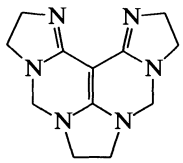
(3aS,4aS,7aS,7bS)-form [117064-12-7]
Reagent for asymmetric induction. $[\alpha]_D$ −339.3° (c, 1.04 in EtOH). Enantiomer also prepd.

[116971-46-1, 117064-10-5, 117064-11-6]

Whitesell, J.K. *et al*, *J. Org. Chem.*, 1988, **53**, 5383 (*synth, resoln, use, abs config*)

2,3,4,5,6,7,8,9,10,11-Decahydro-1,3*a*,5*a*,7*a*,9*a*,12-hexaazatricyclopenta[*a*,*ef*,*j*]heptalene, 9CI D-80011

[111161-01-4]



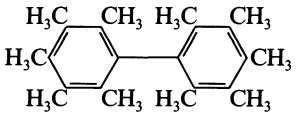
$C_{14}H_{20}N_6$ M 272.352
Mod. sol. aprotic solvs. Mp 228-231°. pK_a 29.22 (MeCN). Mod. stable. Analogues also prepd.

Schwesinger, R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 1165 (*synth, pmr, cryst struct*)

Decamethylbiphenyl D-80012

Permethylbiphenyl

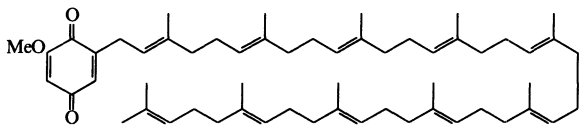
[18356-20-2]



$C_{22}H_{30}$ M 294.479
Mp 239-241°.

Smith, L.I. *et al*, *J. Am. Chem. Soc.*, 1934, **56**, 2169 (*synth*)
Adcock, J.L. *et al*, *J. Organomet. Chem.*, 1974, **72**, 323 (*synth, pmr*)
Biali, S.E. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1917 (*synth*)

2-Decaprenyl-6-methoxy-1,4-benzoquinone D-80013

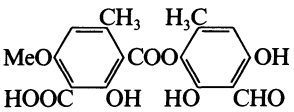


$C_{57}H_{86}O_3$ M 819.305
Isol. from *Rhodospirillum rubrum*. Intermed. in biosynth. of ubiquinones. Not obt. pure.

Friis, P. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 4754.

Decarboxythamnolic acid D-80014

[4356-38-1]



$C_{18}H_{16}O_9$ M 376.319
Detected in *Siphula decumbens* and in *Alectoria* sp. Prisms (Me_2CO). Mp 225°.

Asahina, Y. *et al*, *Ber.*, 1936, **69**, 330; 1939, **72**, 1402 (*synth*)
Bendz, G. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1250.
Solberg, Y., *Acta Chem. Scand., Ser. B*, 1975, **29**, 145 (*isol*)

2,5,8-Decatriene-1,10-diol D-80015

$HOCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2OH$

$C_{10}H_{16}O_2$ M 168.235

(Z,Z,Z)-form [115482-90-1]
Oil. $Bp_{0.01}$ 142°.

Bis(4-methylbenzenesulfonyl): [115482-91-2].
Yellowish oil.

Brudermüller, M. *et al*, *Chem. Ber.*, 1988, **121**, 2255 (*synth, ir, pmr*)

2,5,8-Decatriyne-1,10-diol D-80016

[13002-25-0]

$HOCH_2C{\equiv}CCH_2C{\equiv}CCH_2C{\equiv}CCH_2OH$

$C_{10}H_{10}O_2$ M 162.188
Pale brownish powder ($CHCl_3$/pentane). Mp 109°.

Brudermüller, M. *et al*, *Chem. Ber.*, 1988, **121**, 2255 (*synth*)

4-Decenoic acid D-80017

Updated Entry replacing D-00185

[26303-90-2]

$H_3C(CH_2)_4CH{=}CHCH_2CH_2COOH$

$C_{10}H_{18}O_2$ M 170.251

(E)-form
Bp_{13} 145-146°.

(Z)-form [505-90-8]
Obtusilic acid
Constit. of seed oil of *Lindera obtusiloba* and *L. umbellata*. Bp_{13} 148-150°.

4-Bromophenacyl ester: Mp 43.3°.

Komori, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1937, **12**, 226, 433 (*isol*)
Iwakiri, M., *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1951, **78**, 1460; *ca*, **53**, 21633 (*synth, config*)
Hopkins, C.Y. *et al*, *Lipids*, 1966, **1**, 118 (*isol*)
Bus, J. *et al*, *Chem. Phys. Lipids*, 1976, **17**, 501 (*cmr*)
Furukawa, K. *et al*, *Yukagaku*, 1976, **25**, 190, 358 (*isol*; 296 (*glc, ms, ir, nmr*)

6-Decen-1-ol D-80018

$H_3CCH_2CH_2CH{=}CH(CH_2)_4CH_2OH$

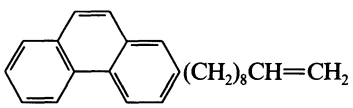
$C_{10}H_{20}O$ M 156.267

(E)-form [38421-92-0]
Liq. $Bp_{0.8}$ 78-79°.

(Z)-form [68760-59-8]
Liq. $Bp_{0.3}$ 74-6°.

Svirskaya, P.I. *et al*, *J. Chem. Eng. Data*, 1979, **24**, 152 (*synth, ir, pmr*)
Brown, H.C. *et al*, *J. Org. Chem.*, 1988, **53**, 246 (*synth, ir, pmr, cmr*)

2-(9-Decenyl)phenanthrene D-80019



$C_{24}H_{28}$ M 316.485
Constit. of *Bryophyllum pinnatum*.

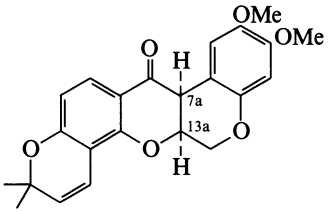
Siddiqui, S. *et al*, *Phytochemistry*, 1989, **28**, 2433 (*isol, pmr, ms*)

Deguelin D-80020

Updated Entry replacing D-20021

*13,13a-Dihydro-9,10-dimethoxy-3,3-dimethyl-3*H-*bis[1]benzopyrano[3,4-*b*:6′,5′-*e*]pyran-7(7a*H*)one, 9CI. Isodeguelin*

[522-17-8]



$C_{23}H_{22}O_6$ M 394.423

CA numbering shown. Isol. from *Crotalaria burhia, Derris elliptica, D. malaccensis, Lonchocarpus* spp., *Millettia ferruginea, M. pachycarpa, Mundulea sericea, Piscidia mollis* and *Tephrosia*spp. (all Leguminosae, Papilionoideae). Cryst. (EtOH). Mp 171°.

▷ Strong irritant, toxic by inhalation.

7a,13a-Didehydro: ***Dehydrodeguelin***

$C_{23}H_{20}O_6$ M 392.407

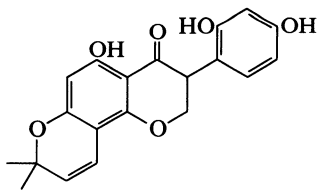
Isol. from *Amorpha fruticosa, D. elliptica, Millettia dura, T. candida* and *T. vogelii*. Yellow cryst. or thick yellow prisms ($CHCl_3$/MeOH). Mp 232-233° (217°).

Clark, E.P. *et al, J. Am. Chem. Soc.*, 1933, **55**, 422 (*Dehydrodeguelin*)
Merz, K.W. *et al, Arch. Pharm.* (*Weinheim, Ger.*), 1935, **273**, 1 (*Dehydrodeguelin*)
Fukami, H. *et al, Agric. Biol. Chem.*, 1961, **25**, 252 (*synth*)
Carlson, D.G. *et al, Tetrahedron*, 1973, **29**, 2731 (*pmr*)
Omokawa, H. *et al, Agric. Biol. Chem.*, 1974, **38**, 1731 (*synth*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Crombie, L. *et al, J. Chem. Soc., Chem. Commun.*, 1986, 352 (*biosynth*)
Begley, M.J. *et al, J. Chem. Soc., Chem. Commun.*, 1986, 353 (*biosynth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 537.

1″,2″-Dehydrocyclokievitone D-80021

*3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5-hydroxy-8,8-dimethyl-4*H,*8*H-*benzo[1,2-*b*:3,4-*b′*]dipyran-4-one, 9CI*

[74175-82-9]



$C_{20}H_{18}O_6$ M 354.359

Tentative struct. Isol. from pods of *Phaseolus vulgaris*.

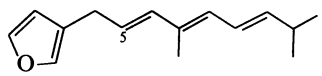
Woodward, M.D., *Phytochemistry*, 1979, **18**, 2007 (*isol, uv, pmr, ms*)

Dehydrodendrolasin D-80022

Updated Entry replacing D-00234

3-(4,8-Dimethyl-2,4,6-nonatrienyl)furan

[41060-02-0]



$C_{15}H_{20}O$ M 216.322

Constit. of *Pleraphysilla spinifera*. Oil.

5Z-Isomer: [117569-45-6].

$C_{15}H_{20}O$ M 216.322

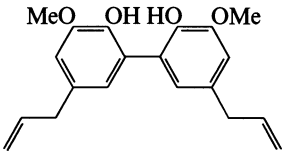
Constit. of *Ceratosoma brevicaudata*. Oil. Reg. no. refers to (*Z,Z,E*) isomer, apparently incorrectly.

Cimino, G. *et al, Tetrahedron*, 1972, **28**, 4761 (*isol, struct*)
Ksebati, M.B. *et al, J. Nat. Prod.* (*Lloydia*), 1988, **51**, 857 (*isol, struct, pmr, cmr*)

Dehydrodieugenol D-80023

3,3′-Dimethoxy-5,5′-di-2-propenyl[1,1′-biphenyl]-2,2′-diol, 9Cl. 5,5′-Diallyl-2,2′-dihydroxy-3,3′-dimethoxybiphenyl. $\Delta^{8,8'}$-4,4′-Dihydroxy-5,5′-dimethoxy-3,3′-neolignan. Bieugenol

[4433-08-3]



$C_{20}H_{22}O_4$ M 326.391

Isol. from Java citronella oil, from *Litsea turfosa, Ocotea cymbanum, Virola carinata and Nectandra polita*. Tablets (EtOH). Mp 106°.

Mono-Me ether: [75225-84-2]. ***O-Methyldehydrodieugenol***

$C_{21}H_{24}O_4$ M 340.418

Isol. from *O. cymbanum, V. carinata and N. polita*. Oil.

Di-Me ether: [13417-56-6]. ***Dimethyldehydrodieugenol***

$C_{22}H_{26}O_4$ M 354.445

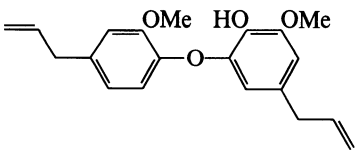
Isol. from *N. polita*. Oil.

Jones, H.A. *et al, J. Am. Chem. Soc.*, 1940, **62**, 2558 (*isol*)
Holloway, D.M. *et al, Phytochemistry*, 1973, **12**, 1503 (*isol*)
de Diaz, A.M.P. *et al, Phytochemistry*, 1980, **19**, 681 (*isol*)
Kawanishi, K. *et al, Phytochemistry*, 1981, **20**, 1166 (*isol, pmr, deriv*)
Suarez, M. *et al, Phytochemistry*, 1983, **22**, 609 (*isol, cmr, derivs*)

Dehydrodieugenol B D-80024

2-Methoxy-6-[2-methoxy-4-(2-propenyl)phenoxy]-4-(2-propenyl)phenol, 9CI. 4′,5-Diallyl-2-hydroxy-2′,3-dimethoxybiphenyl ether

[75225-33-1]



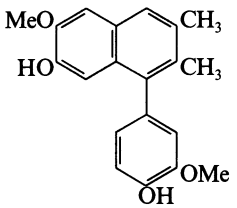
$C_{20}H_{22}O_4$ M 326.391

Isol. from trunkwood of *Octotea cymbarum*. Oil.

de Diaz, A.M.P. *et al, Phytochemistry*, 1980, **19**, 681 (*isol, uv, ir, pmr, ms, struct*)

Dehydroguaiaretic acid D-80025

8-(4-Hydroxy-3-methoxyphenyl)-3-methoxy-6,7-dimethyl-2-naphthol



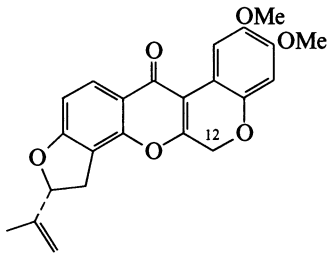
$C_{20}H_{20}O_4$ M 324.376
Minor constit. of wood of *Guaiacum officinale*.
Di-Et ester: Prisms (EtOAc). Mp 162-163°.

King, F.E. *et al*, *J. Chem. Soc.*, 1964, 4011 (*isol, uv, synth*)

Dehydrorotenone D-80026

*1,2-Dihydro-8,9-dimethoxy-2-(1-methylethenyl)[1]benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(12*H*)one, 9CI. Didehydrorotenone*

[30990-44-4]



$C_{23}H_{20}O_6$ M 392.407

(R)-form [3466-09-9]
Isol. from *Derris elliptica, D. ferruginea, D. negrensis, D. uliginosa Lonchocarpus longifolius, L. urucu, Millettia ferruginea, M. pachycarpa, Mundulea sericea, Neorautanenia amboensis, Tephrosia falciformis* and *T. virginiana*. Pale yellow cryst. (C_6H_6/pet. ether). Mp 212-213°. $[\alpha]_D$ −27.5° (c, 0.8 in $CHCl_3$).

12-Hydroxy: [57103-58-9]. ***Amorpholone***
$C_{23}H_{20}O_7$ M 408.407
Constit. of the roots of *Amorpha canescens*. Yellow needles ($CHCl_3$). Mp 255-260°. No opt. rotn. or chirality reported.

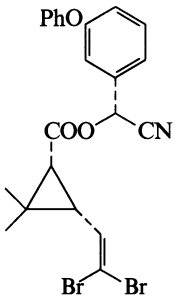
12-Oxo: [4439-62-7]. ***Rotenonone***
$C_{23}H_{18}O_7$ M 406.391
Isol. from *A. canescens* and *N. amboensis*. Bright-yellow needles (dichloroethane). Mp 295-308° dec.

Piatak, D.M. *et al*, *Phytochemistry*, 1975, **14**, 1391 (*Amorpholone*)
Bose, P.C. *et al*, *Indian J. Chem., Sect. B*, 1976, **14**, 1012 (*isol, uv, ms, struct*)
Oberholzer, M.E. *et al*, *Phytochemistry*, 1976, **15**, 1283 (*Rotenonone*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*occur*)

Deltamethrin D-80027

3-(2,2-Dibromoethenyl)-2,2-dimethylcyclopropanecarboxylic acid cyano(3-phenoxyphenyl)methyl ester, 9CI. Decamethrin. Decis. K-Othrine. Butox. Butoflin

[52918-63-5]

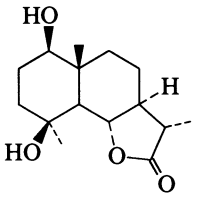


Absolute configuration

$C_{22}H_{19}Br_2NO_3$ M 505.205
Potent, photostable pyrethroid used as contact and stomach poison against a wide range of insects. Powder. Mp 100°. $[\alpha]_D$ +61° (c, 4 in C_6H_6).

Elliott, M. *et al*, *Nature (London)*, 1974, **248**, 710 (*synth, pmr*)
Lidgurd, R.O. *et al*, *Biomed. Mass Spectrom.*, 1986, **13**, 677; *CA*, **106**, 133627p (*ms*)
Pesticide Manual, 8th Ed., 1987, 3890.

Dendroserin D-80028



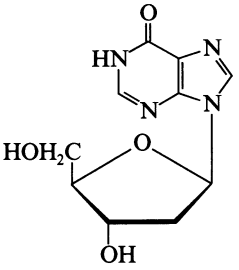
$C_{15}H_{24}O_4$ M 268.352
Constit. of *Dendroseris neriifolia*. Needles (MeOH). Mp 178-182°.

Campos, V. *et al*, *Heterocycles*, 1989, **28**, 779.

2′-Deoxyinosine D-80029

9-(2-Deoxyribofuranosyl)hypoxanthine. Hypoxanthine 2-deoxyriboside

[29868-32-4]

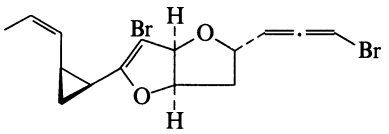


$C_{10}H_{12}N_4O_4$ M 252.229
Isol. from herring sperm DNA, from *Phaseolus vulgaris, Laminaria saccharina, Furcellaria fastigiata, Lactobacillus* spp. etc. Needles (MeOH). Mp 218° dec. $[\alpha]_D^{27}$ +7.92° (c, 0.53 in 0.1M NaOH).

Manson, L.A. *et al*, *J. Biol. Chem.*, 1951, **191**, 87 (*isol*)
Banhidi, Z.G. *et al*, *Acta Chem. Scand.*, 1953, **7**, 713 (*isol*)
Venner, H., *Chem. Ber.*, 1960, **93**, 140 (*synth*)
Robins, M.J. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 4934 (*pmr*)
Rousseau, R.J. *et al*, *J. Heterocycl. Chem.*, 1970, **7**, 367 (*synth, uv*)

Deoxyokamurallene D-80030

Updated Entry replacing D-10036

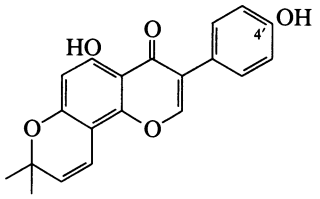


$C_{15}H_{16}Br_2O_2$ M 388.098
Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{23}$ +220° (c, 0.84 in $CHCl_3$).

Suzuki, M. *et al*, *Chem. Lett.*, 1982, 289 (*isol*)
Suzuki, M. *et al*, *Phytochemistry*, 1989, **28**, 2145 (*struct*)

Derrone D-80031

*5-Hydroxy-3-(4-hydroxyphenyl)-8,8-dimethyl-4*H,*8*H-*benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, 9CI*
[76166-59-1]

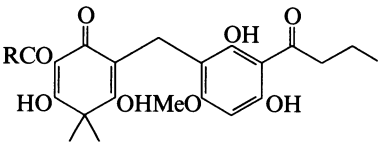


$C_{20}H_{16}O_5$ M 336.343
Isol. from seeds of *Derris robusta*. Cryst. Mp 216-218°.
Di-Ac: Needles. Mp 225-227°.
4′-O-Me: [34086-52-7]. ***4′-O-Methylderrone***
$C_{21}H_{18}O_5$ M 350.370
Isol. from *D. robusta* and from *Calopogonium mucunoides*. Mp 170-172°.

Jackson, B. *et al*, *J. Chem. Soc. C*, 1971, 3389 (*synth, deriv*)
Vilain, C. *et al*, *Bull. Soc. R. Sci. Liege*, 1975, **44**, 306; *CA*, **84**, 74136e (*isol, deriv*)
Chibber, S.S., *Phytochemistry*, 1980, **19**, 1857 (*isol, uv, pmr*)

Desaspidins D-80032

Updated Entry replacing D-00465



Desaspidin AB, R = CH_3
PB, R = CH_2CH_3
BB, R = $CH_2CH_2CH_3$

The alphabetical suffixes refer to the acyl chains (A = acetyl, P = propionyl, B = butyryl). Isol. from male ferns *Dryopteris* spp.

▷ EU1225000.

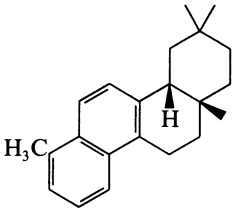
Desaspidin AB [3572-07-4]
$C_{22}H_{26}O_8$ M 418.443
Cryst. (cyclohexane). Mp 145-147° (synthetic).

Desaspidin PB
$C_{23}H_{28}O_8$ M 432.469
Mp 141-142° (synthetic).

Desaspidin BB [114-43-2]
Desapidin. Resapin
$C_{24}H_{30}O_8$ M 446.496
Anthelmintic. Cryst. (Et_2O/pet. ether). Mp 150-150.5°.

Aebi, A. *et al*, *Helv. Chim. Acta*, 1957, **40**, 266 (*isol*)
Penttilä, A. *et al*, *Acta Chem. Scand.*, 1964, **18**, 344 (*isol, synth*)
Lounasmaa, M. *et al*, *Acta Chem. Scand.*, 1972, **26**, 89 (*ms*)
Widen, C.J. *et al*, *Helv. Chim. Acta*, 1975, **58**, 880; 1976, **59**, 1725 (*isol, bibl*)
Ayras, P. *et al*, *Org. Magn. Reson.*, 1981, **16**, 209 (*cmr*)
Martindale, *The Extra Pharmacopoeia*, 28th/29th Eds., Pharmaceutical Press, London, 1982/1989, 770.

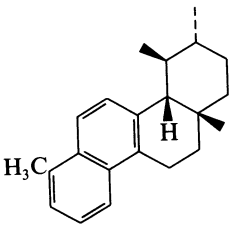
Des-A-26,27-dinoroleana-5,7,9,11,13-pentaene D-80033



$C_{22}H_{28}$ M 292.463
Constit. of surface sediments.

Trendel, J.M. *et al*, *Tetrahedron*, 1989, **45**, 4457.

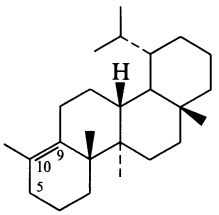
Des-A-26,27-dinor-5,7,9,11,13-ursapentaene D-80034



$C_{22}H_{28}$ M 292.463
Constit. of surface sediments.

Trendel, J.M. *et al*, *Tetrahedron*, 1989, **45**, 4457.

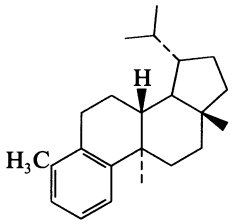
Des-A-lup-9-ene D-80035



$C_{24}H_{40}$ M 328.580
Constit. of surface sediments. Cryst. ($MeOH/CH_2Cl_2$). Mp 117.5°. $[\alpha]_D$ −107° (c, 0.586 in $CHCl_3$).
9α,10β-Dihydro: ***10β*H-*Des-A-lupane***
$C_{24}H_{42}$ M 330.596
Constit. of surface sediments. Cryst. ($MeOH/CH_2Cl_2$). Mp 94-95°.
$\Delta^{5(10)}$-*Isomer:* ***Des-A-lup-5(10)-ene***
$C_{24}H_{40}$ M 328.580
Constit. of surface sediments. Cryst. ($MeOH/CH_2Cl_2$). Mp 174°.

Corbet, B. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 1171 (*synth*)
Trendel, J.M. *et al*, *Tetrahedron*, 1989, **45**, 4457 (*isol, synth, cryst struct*)

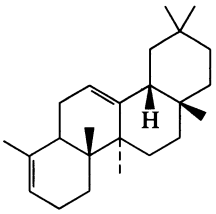
Des-A-26-nor-5,7,9-lupatriene D-80036



$C_{23}H_{34}$ M 310.522
Constit. of sediments.

Wolff, G.A. *et al*, *Tetrahedron*, 1989, **45**, 6721 (*synth*)

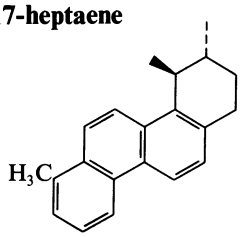
Des-A-5(10),12-oleanadiene D-80037



$C_{24}H_{38}$ M 326.564
Constit. of surface sediments.

Trendel, J.M. *et al*, *Tetrahedron*, 1989, **45**, 4457.

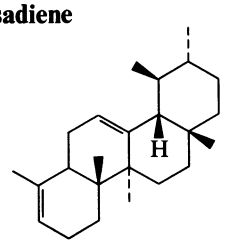
Des-A-26,27,28-trisnorursa-5,7,9,11,13,15,17-heptaene D-80038



$C_{21}H_{22}$ M 274.405
Constit. of surface sediments. Cryst. ($MeOH/CH_2Cl_2$).

Trendel, J.M. *et al*, *Tetrahedron*, 1989, **45**, 4457 (*cryst struct*)

Des-A-5(10),12-ursadiene D-80039

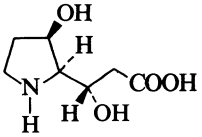


$C_{24}H_{38}$ M 326.564
Constit. of surface sediments.

Trendel, J.M. *et al*, *Tetrahedron*, 1989, **45**, 4457.

Detoxinine D-80040

Updated Entry replacing D-20037



$C_7H_{13}NO_4$ M 175.184

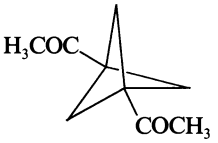
(−)-*form*
Structural component of Detoxin D_1, D-00484. $[\alpha]_D^{23}$ −4.1° (c, 0.5 in H_2O).

(±)-*form*
Prisms. Mp >200° dec.

Haüsler, J., *Justus Liebigs Ann. Chem.*, 1983, 982 (*synth*)
Ohfune, Y. *et al*, *Tetrahedron Lett.*, 1984, **25**, 4133 (*synth*)
Ewing, W.R. *et al*, *Tetrahedron*, 1986, **42**, 2421 (*synth, ir, pmr*)

1,3-Diacetylbicyclo[1.1.1]pentane D-80041

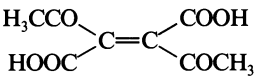
[115913-30-9]



$C_9H_{12}O_2$ M 152.193
Cryst. (heptane). Mp 67-69°.

Kaszynski, P. *et al*, *J. Org. Chem.*, 1988, **53**, 4593 (*synth, pmr, cmr, ir, ms*)

2,3-Diacetyl-2-butenedioic acid, 9CI D-80042



(*E*)-*form*

$C_8H_8O_6$ M 200.148

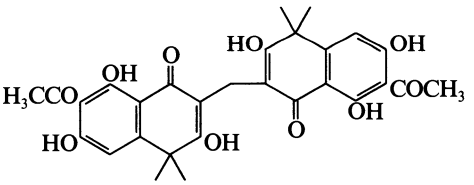
(*E*)-*form*

Di-Et ester: [69622-58-8]. *Diethyl diacetylfumarate*
$C_{12}H_{16}O_6$ M 256.255
Needles (Et_2O). Mp 93-95°. Readily cyclises.

[69622-59-9, 92236-43-6]

Adembri, G. *et al*, *Gazz. Chim. Ital.*, 1983, **113**, 489.

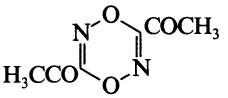
Di-2-(7-acetyl-1,4-dihydro-3,6,8-trihydroxy-4,4-dimethyl-1-oxonaphthyl) methane D-80043



$C_{29}H_{28}O_{10}$ M 536.534
Pigment from root of *Cassia semicordata*. Cryst. Mp 266-267°.

Delle Monache, G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 6203.

3,6-Diacetyl-1,4,2,5-dioxadiazine D-80044



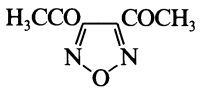
$C_6H_6N_2O_4$ M 170.124

Dioxime: [116303-45-8]. *Schmitz's compound*
$C_6H_8N_4O_4$ M 200.154
Cryst. (EtOH). Mp 191°.

Fruttero, R. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 1017 (*struct, cmr, N-15 nmr, bibl*)

3,4-Diacetylfurazan D-80045

1,1′-(3,4-Furazandiyl)bisethanone, 9CI



$C_6H_6N_2O_3$ M 154.125
Oil.

N-*Oxide:* [6103-08-8]. *3,4-Diacetylfuroxan*
$C_6H_6N_2O_4$ M 170.124
Yellow oil. Bp_1 100°.
▷ Explodes on dist. unless pure.

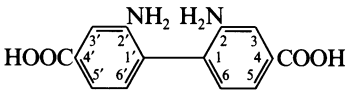
N-*Oxide, dioxime*(E,E-): [116303-46-9]. *3,4-Diacetylfuroxan dioxime. Tryller's compound*
$C_6H_8N_4O_4$ M 200.154
Cryst. ($CHCl_3$). Mp 145°.

Peterson, L.I., *Tetrahedron Lett.*, 1966, 1727 (*synth, oxide, pmr*)
Fruttero, R. *et al, Justus Liebigs Ann. Chem.*, 1988, 1017 (*struct, cmr, N-15 nmr, bibl*)

2,2′-Diamino-4,4′-biphenyldicarboxylic acid D-80046

2,2′-Diamino-4,4′-diphenic acid

[41738-56-1]



$C_{14}H_{12}N_2O_4$ M 272.260
Yellow platelets (EtOH or H_2O). Mp 307-309°.

Di-Me ester: [23933-57-5].
$C_{16}H_{16}N_2O_4$ M 300.313
Mp 174-176°.

Di-Et ester:
$C_{18}H_{20}N_2O_2$ M 296.368
Needles or pale-yellow scales. Mp 99-100°, Mp 112-115° (dimorph.).

N,N′-Di-Ac:
$C_{18}H_{16}N_2O_6$ M 356.334
Mp 250°.

Jakubowski, Z. *et al, Ber.*, 1909, **42**, 634.
Adams, R. *et al, J. Am. Chem. Soc.*, 1933, **55**, 1649.
Cheung King Ling, C., *J. Chem. Soc.*, 1964, 1825.

4,4′-Diamino-2,2′-biphenyldicarboxylic acid D-80047

4,4′-Diaminodiphenic acid, 8CI. Benzidine-2,2′-dicarboxylic acid

[17557-76-5]

$C_{14}H_{12}N_2O_4$ M 272.260
Polymer intermediate. Needles. Mp 265°.

Anhydride, N,N′-*Di-Ac:*
$C_{18}H_{14}N_2O_5$ M 338.319
Needles (Ac_2O). Mp >300°.

Schmidt, J. *et al, Ber.*, 1905, **28**, 3771 (*synth*)
Adkins, H. *et al, J. Am. Chem. Soc.*, 1917, **46**, 1924 (*synth*)
Patel, H.R. *et al, J. Am. Pharm. Assoc.*, 1957, **46**, 51 (*synth*)

4,4′-Diamino-2,3′-biphenyldicarboxylic acid D-80048

Benzidine-2,3′-dicarboxylic acid

$C_{14}H_{12}N_2O_2$ M 240.261

Paal, C. *et al, Ber.*, 1892, **25**, 3590.

4,4′-Diamino-3,3′-biphenyldicarboxylic acid D-80049

Benzidine-3,3′-dicarboxylic acid

[2130-56-5]

$C_{14}H_{12}N_2O_4$ M 272.260
Polymer intermed. Needles. Mp 300° (275°) dec.
▷ Weak carcinogen.

N,N′-Di-Ac:
$C_{18}H_{16}N_2O_6$ M 356.334
Mp 300° (unsharp).

N,N′-Dibenzoyl:
$C_{28}H_{20}N_2O_6$ M 480.476
Mp 302-304°.

Diamide: [15420-64-1].
$C_{14}H_{14}N_4O_4$ M 302.289
Mp 340°.

Bülow, C. *et al, Ber.*, 1898, **31**, 2574 (*derivs*)
Schultz, G. *et al, Justus Liebigs Ann. Chem.*, 1907, **352**, 111 (*synth*)
Pliss, G.B., *CA*, 1969, **71**, 48193h (*tox*)
Rabilloud, G. *et al, J. Heterocycl. Chem.*, 1980, **17**, 1065 (*synth*)
Niume, K. *et al, J. Polym. Sci., Part A*, 1981, **19**, 1745 (*synth*)

4,6′-Diamino-2,2′-biphenyldicarboxylic acid D-80050

4,6′-Diaminodiphenic acid, 8CI

[67003-04-7]

$C_{14}H_{12}N_2O_4$ M 272.260
Needles. V. insol. org. solvs. Mp 327-330° dec. (312-313°).

Schad, P., *Ber.*, 1893, **26**, 216 (*synth*)
Adkins, H. *et al, J. Am. Chem. Soc.*, 1917, **46**, 1924 (*synth*)
Patel, H.R. *et al, J. Am. Pharm. Assoc.*, 1957, **46**, 51 (*synth*)

5,5′-Diamino-2,2′-biphenyldicarboxylic acid D-80051

5,5′-Diaminodiphenic acid

$C_{14}H_{12}N_2O_2$ M 240.261
Mp 265° dec.

Di-Me ester:
$C_{16}H_{16}N_2O_2$ M 268.315
Mp 220-222°.

N,N′-Di-Ac:
$C_{18}H_{16}N_2O_4$ M 324.335
Mp >300° (darkens).

Pufahl, F., *Ber.*, 1929, **62**, 2817.

6,6′-Diamino-2,2′-biphenyldicarboxylic acid D-80052

6,6′-Diamino-2,2′-diphenic acid. 2,7-Diaminodiphenic acid (obsol.)

$C_{14}H_{12}N_2O_4$ M 272.260

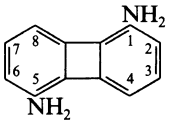
(±)-***form***
Mp 265° (250-251°).

Adkins, H. *et al, J. Am. Chem. Soc.*, 1924, **46**, 1917 (*synth*)

1,5-Diaminobiphenylene D-80053

1,5-Biphenylenediamine, 9CI

[17532-90-0]



$C_{12}H_{10}N_2$ M 182.224

Pale yellow needles (MeOH). Mp 233-235°.

Iqbal, K. *et al*, *J. Chem. Soc. C*, 1967, 1690 (*synth, pmr*)

2,3-Diaminobiphenylene D-80054

2,3-Biphenylenediamine

[32281-46-2]

$C_{12}H_{10}N_2$ M 182.224

Yellow-brown plates (C_6H_6/hexane). Mp 198-200° subl.

N,N'-Di-Ac: [32281-47-3].

$C_{16}H_{14}N_2O_2$ M 266.299

Pale yellow needles (MeOH). Mp 285-287°.

Barton, J.W. *et al*, *J. Chem. Soc. C*, 1971, 1384 (*synth, deriv*)

2,6-Diaminobiphenylene D-80055

2,6-Biphenylenediamine

[70468-22-3]

$C_{12}H_{10}N_2$ M 182.224

Polymer intermediate. Deep yellow plates (pet. ether). Mp 218-220° dec.

N,N'-Di-Ac:

$C_{16}H_{14}N_2O_2$ M 266.299

Orange needles (EtOH). Mp 328-330° dec.

Baker, W. *et al*, *J. Chem. Soc.*, 1960, 414 (*synth, deriv, uv*)
Swedo, R.J. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1978, **16**, 2711 (*synth*)

1,8-Diaminocarbazole D-80056

9H-Carbazole-1,8-diamine

[117110-85-7]

$C_{12}H_{11}N_3$ M 197.239

Silver plates (C_6H_6). Mp 230° dec.

1,8-N-Di-Ac:

$C_{16}H_{15}N_3O_2$ M 281.313

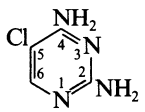
Needles (EtOH). Mp 320-322° dec.

Takahashi, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1869 (*synth, ir, pmr*)

2,4-Diamino-5-chloropyrimidine, 8CI D-80057

5-Chloro-2,4-pyrimidinediamine, 9CI

[18620-64-9]



$C_4H_5ClN_4$ M 144.563

Cryst. (H_2O). Mp 200-202°. pK_a 5.58.

3-Oxide: [91481-97-9].

$C_4H_5ClN_4O$ M 160.562

Cryst. (EtOH). Mp 222-224°. pK_a 1.99.

Roth, B. *et al*, *J. Org. Chem.*, 1969, **34**, 821 (*uv*)
Cowden, W.B. *et al*, *Aust. J. Chem.*, 1979, **32**, 2049; 1984, **37**, 1195 (*synth, props, uv, oxide*)

2,4-Diamino-6-chloropyrimidine, 8CI D-80058

6-Chloro-2,4-pyrimidinediamine, 9CI

[156-83-2]

$C_4H_5ClN_4$ M 144.563

Cryst. (Me_2CO). Mp 200-201°. pK_a 3.57.

▷ Irritant.

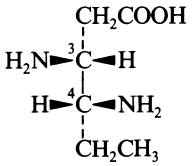
3-Oxide: [35139-67-4].

$C_4H_5ClN_4O$ M 160.562

Cryst. (EtOH). Mp 190° dec. pK_a 2.25.

Aldrich Library of IR Spectra, No.1363A.
Aldrich Library of NMR Spectra, 2nd Ed., **2**, 703D.
Hull, R. *et al*, *J. Chem. Soc.*, 1947, 41 (*synth*)
Roth, B. *et al*, *J. Org. Chem.*, 1969, **34**, 821 (*uv*)
Delia, T.J. *et al*, *J. Heterocycl. Chem.*, 1972, **9**, 73 (*oxide, synth, pmr, uv*)
Staedeli, W. *et al*, *Helv. Chim. Acta*, 1980, **63**, 504 (*N*-15 *nmr*)
Cowden, W.B. *et al*, *Aust. J. Chem.*, 1984, **37**, 1195 (*props, oxide, synth, pmr, uv*)

3,4-Diaminohexanoic acid D-80059



(3*R*,4*R*)-*form*

$C_6H_{14}N_2O_2$ M 146.189

(3*R*,4*R*)-*form* [120452-75-7]

N^3-tert-*Butyloxycarbonyl:* Cryst. (MeOH/Et_2O). $[\alpha]_D^{20}$ +7.0° (c, 0.9 in MeOH).

(3*R*,4*S*)-*form* [120452-77-9]

N^3-tert-*Butyloxycarbonyl:* Cryst. (MeOH/Et_2O). Mp 151-153°. $[\alpha]_D^{20}$ + ±0.0° (c, 1.0 in MeOH). Incorr. descr. as (3*R*,4*R*).

Kano, S. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3341 (*synth, pmr*)

5,6-Diaminohexanoic acid D-80060

δ-Lysine

$H_2NCH_2CH(NH_2)CH_2CH_2CH_2COOH$

$C_6H_{14}N_2O_2$ M 146.189

(±)-*form*

B,2HCl: [118894-93-2].

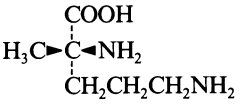
Mp 163° dec.

Altman, J. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 493 (*synth, pmr*)

2,5-Diamino-2-methylpentanoic acid D-80061

2-Methylornithine, 9CI

[48047-94-5]



(*R*)-*form*

$C_6H_{14}N_2O_2$ M 146.189

(*R*)-*form* [59574-27-5]

D-*form*

Mp 197-199° dec. $[\alpha]_D$ −10.21° (c, 0.7 in 4M HCl).

B,HCl: Mp 214°. $[\alpha]_D^{20}$ −10° (c, 1 in H_2O).

(*S*)-*form* [48047-95-6]

L-*form*

B,HCl: [59545-84-5].

Cryst. (EtOH aq.). Mp 218°. $[\alpha]_D^{20}$ +8.4° (c, 0.5 in H_2O).

(±)-*form*

Potent reversible inhibitor of ornithine decarboxylase.

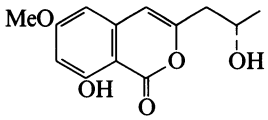
B,HCl: Cryst. + $1H_2O$ (Me_2CO aq.). Dehydrates at 250°.

Abdel-Monem, M.M. *et al*, *J. Med. Chem.*, 1974, **17**, 447.
Bey, P. *et al*, *J. Med. Chem.*, 1978, **21**, 50 (*synth, abs config*)
Gander-Coquoz, M. *et al*, *Helv. Chim. Acta*, 1988, **71**, 224 (*synth, ir, pmr, ms*)

Diaporthin D-80062

Updated Entry replacing D-70050

8-Hydroxy-3-(2-hydroxypropyl)-6-methoxy-1H-2-benzopyran-1-one, 9CI. 8-Hydroxy-3-(2-hydroxypropyl)-6-methoxyisocoumarin



$C_{13}H_{14}O_5$ M 250.251

(*S*)-*form* [10532-39-5]

Isol. from cultures of *Endothia parasitica*. Phytotoxin. Needles or plates. Mp 90-92° (83-85°). $[\alpha]_D$ +54° (c, 10.87 in $CHCl_3$).

O-*De-Me:* ***Orthosporin.*** *De-O-methyldiaporthin*

$C_{12}H_{12}O_5$ M 236.224

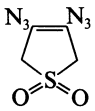
Phytotoxin from *Drechslera siccans* and *Rhynchosporium orthosporum*. Needles. Mp 183-184°. $[\alpha]_D^{22}$ +61.8° (c, 1 in MeOH).

Hardegger, E. *et al*, *Helv. Chim. Acta*, 1966, **49**, 1283 (*isol, props*)
Hallock, Y.F. *et al*, *Phytochemistry*, 1988, **27**, 3123 (*isol*)
Ichihara, A. *et al*, *Chem. Lett.*, 1989, 1495 (*struct, synth, abs config*)

3,4-Diazido-3,5-dihydro-thiophene 1,1-dioxide D-80063

3,4-Diazido-3-sulfolene

[114397-29-4]



$C_4H_4N_6O_2S$ M 200.181

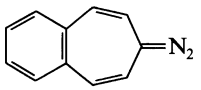
Yellow solid. Mp 82-83.5°. Gradually dec. on standing.

Chou, T. *et al*, *J. Org. Chem.*, 1988, **53**, 3027 (*synth, pmr, ir, ms*)

7-Diazo-7*H*-benzocycloheptene, 9CI D-80064

4,5-Benzodiazocycloheptatriene

[111743-26-1]



$C_{11}H_8N_2$ M 168.198

Precursor to the triplet 4,5-benzocycloheptatrienylidene carbene and 4,5-benzocycloheptatrienylradical. Brown solid. Thermally unstable. Could not be cryst.

Chateauneuf, J.E. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 539 (*synth, ir, uv, pmr*)

Diazomethanesulfonic acid D-80065

$N_2{=}CHSO_3H$

$CH_2N_2O_3S$ M 122.104

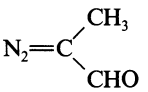
Esters prepd. and characterised spectroscopically.

[120263-45-8, 120263-47-0]

Berkessel, A. *et al*, *Chem. Ber.*, 1989, **122**, 1147.

2-Diazopropanal, 9CI D-80066

[19547-06-9]



$C_3H_4N_2O$ M 84.077

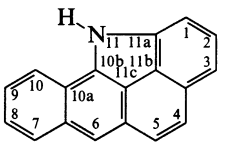
Oil. Bp_{12} 35°.

Regitz, M. *et al*, *Chem. Ber.*, 1968, **101**, 2622 (*synth*)
Kučera, J. *et al*, *Collect. Czech. Chem. Commun.*, 1970, **35**, 3618 (*synth, uv*)
Menicagli, R. *et al*, *Tetrahedron*, 1987, **43**, 171 (*synth, ir, pmr*)

11*H*-Dibenzo[*a,def*]carbazole D-80067

1,12-Iminobenz[a]*anthracene*

[40831-21-8]



$C_{18}H_{11}N$ M 241.292

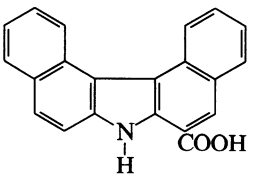
Reg. no. refers to 1*H*-form. Pale-yellow cryst. (C_6H_6). Mp 217-219.5°. Intense blue fluor. in soln.

Picrate: Dark brown needles. Mp 191-192°.

Badger, G.M. *et al*, *J. Chem. Soc.*, 1949, 799.

Dibenzo[*c,g*]carbazole-6-carboxylic acid D-80068

[111960-35-1]



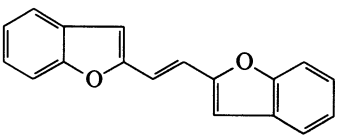
$C_{21}H_{13}NO_2$ M 311.339

Cryst. ($CHCl_3$). Mp 286-288°.

Katritzky, A.R. *et al*, *J. Org. Chem.*, 1988, **53**, 794 (*synth, pmr*)

1,2-Di-(1-Benzofuranyl)ethylene D-80069

2,2'-(1,2-Ethenediyl)bisbenzofuran, 9CI



$C_{18}H_{12}O_2$ M 260.292

(*E*)-*form* [115983-55-6]

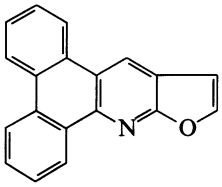
Cryst. (EtOH). Mp 185°.

Capuano, L. *et al*, *Chem. Ber.*, 1988, **121**, 2259 (*synth, pmr, uv*)

Dibenzo[f,*h*]furo[2,3-*b*]quinoline, 9CI **D-80070**

*Phenanthro[9,10-*e*]furo[2,3-*b*]pyridine*

[115170-34-8]



$C_{19}H_{11}NO$ M 269.302

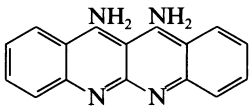
Powder. Mp 161.5-163°.

Taylor, E.C. *et al*, *Tetrahedron*, 1987, **43**, 5145 (*synth, ir, pmr, cmr*)

Dibenzo[*b,g*][1,8]naphthyridine-11,12-diamine, 9CI **D-80071**

11,12-Diaminodibenzo[b,g][*1,8*]*naphthyridine*

[117096-00-1]



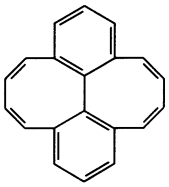
$C_{16}H_{12}N_4$ M 260.298

Yellow solid + $0.4H_2O$ by subl. Mp 314-316°. pK_a 3.3.

Shi, S. *et al*, *J. Org. Chem.*, 1988, **53**, 5379 (*synth, ir, pmr, cmr, ms*)

Dibenzo[f*g,mn*]octalene **D-80072**

[111409-90-6]



$C_{20}H_{14}$ M 254.331

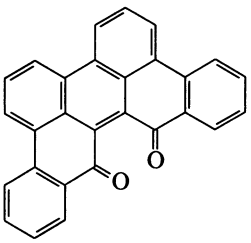
Needles (hexane). Mp 188°.

Heinz, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 1291 (*synth, pmr, cmr, uv*)

Dibenzo[f*g,ij*]pentaphene-15,16-dione, 9CI **D-80073**

2,3:10,11-Dibenzperylene-1,12-quinone (*obsol.*)

[116897-91-7]



$C_{28}H_{14}O_2$ M 382.417

Mp 336° (330°).

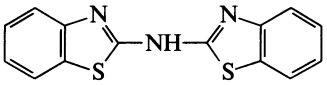
Zinke, A. *et al*, *Ber.*, 1941, **74**, 115 (*synth*)

Hewgill, F.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1305 (*synth, ir, pmr, cmr*)

Di-2-benzothiazolylamine **D-80074**

N-*2-Benzothiazolyl-2-benzothiazolamine*, *9CI. 2,2'-Iminobis*[*benzo-1,3-thiazole*]

[34997-17-6]



$C_{14}H_9N_3S_2$ M 283.377

Cryst. (1-butanol). Mp 256-257°.

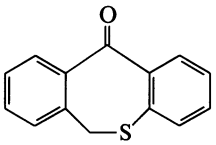
Neidlein, R. *et al*, *Synthesis*, 1971, 540 (*synth*)

Garín, J. *et al*, *Synthesis*, 1987, 368 (*synth, pmr, ms*)

Dibenzo[*b,e*]thiepin-11(6*H*)-one, 9CI **D-80075**

6,11-Dihydrodibenzo[b,e]*thiepin-11-one*

[1531-77-7]



$C_{14}H_{10}OS$ M 226.298

Intermediate in synth. of tranquilizers, antidepressants, antiemetics and antihistamines. Cryst. (EtOH or Et_2O/pet. ether). Mp 86-88°. Bp_1 175-180°.

Stach, K. *et al*, *Angew. Chem.*, 1962, **74**, 31, 752.

Stach, K. *et al*, *Monatsh. Chem.*, 1962, **93**, 889 (*synth, uv, ir, pmr*)

Volanschi, E. *et al*, *Rev. Roum. Chim.*, 1974, **19**, 755; *CA*, **81**, 62865s (*esr*)

Sindelar, K. *et al*, *Collect. Czech. Chem. Commun.*, 1983, **48**, 1898 (*pharmacol*)

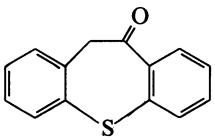
Dolivka, Z. *et al*, *Collect. Czech. Chem. Commun.*, 1985, **50**, 1078; 1987, **52**, 1566 (*use*)

Wyatt, D.K. *et al*, *Appl. Spectrosc.*, 1986, **40**, 369 (*cmr*)

Dibenzo[*b,f*]thiepin-10(11*H*)-one, 9CI **D-80076**

10,11-Dihydrodibenzo[b,f]*thiepin-10-one*

[1898-85-7]



Used in synth. of antidepressants and analgesics. Solid. Mp 72-73°.

*Org. Synth., Coll.Vol.*1, 552 (*synth*)

Jelek, J.O. *et al*, *Monatsh. Chem.*, 1965, **96**, 182 (*synth, ir*)

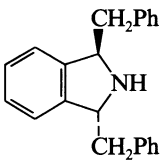
Ueda, I., *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2306 (*synth*)

Sindelar, K. *et al*, *Collect. Czech. Chem. Commun.*, 1983, **48**, 1187 (*synth*)

1,3-Dibenzyl-1,3-dihydroisoindole **D-80077**

*2,3-Dihydro-1,3-bis(phenylmethyl)-1*H*-isoindole*, *9CI. 1,3-Dibenzylisoindoline*

[117185-28-1]



$C_{22}H_{21}N$ M 299.415

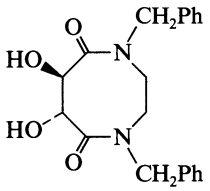
(***R,R***)-*form*

Reagent for asymmetric synthesis. $[\alpha]_D$ −5.4° (c, 2.15 in EtOH).

Gawley, R.E. *et al*, *J. Org. Chem.*, 1988, **53**, 5381 (*synth, pmr*)

1,4-Dibenzyl-6,7-dihydroxy-1,4-diazocane-5,8-dione D-80078

1,2,3,4,6,7-Hexahydro-6,7-dihydroxy-1,4-bis(phenylmethyl)-1,4-diazocine-5,8-dione, 9CI. N,N′-*Dibenzyl*-N,N′-*ethylenetartramide*



(*R,R*)-*form*

$C_{20}H_{22}N_2O_4$ M 354.405

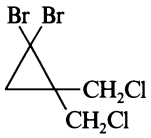
(***R,R***)-***form*** [112897-01-5]

Chiral auxiliary for allylboronation. Cryst. (EtOH aq.). Mp 202-203°. $[\alpha]_D^{25}$ −73.9° (c, 1 in dioxan).

Roush, W.R. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3979 (*synth, pmr, ir, use*)

1,1-Dibromo-2,2-bis(chloromethyl) cyclopropane D-80079

[98577-44-7]



$C_5H_6Br_2Cl_2$ M 296.816

Cryst. (Et_2O). Mp 45-46°.

Belzner, J. *et al*, *Chem. Ber.*, 1989, **122**, 397 (*synth, pmr, cmr, ms*)

2,4-Dibromobutanoic acid D-80080

[63164-16-9]

$BrCH_2CH_2CHBrCOOH$

$C_4H_6Br_2O_2$ M 245.898

(±)-***form***

Bp_{15} 130-131°.

Chloride: [82820-87-9].

$C_4H_5Br_2ClO$ M 264.344

Bp_1 60-75°.

Amide: [54882-37-0].

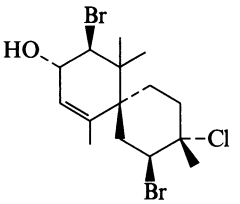
$C_4H_7Br_2NO$ M 244.913

Solid.

Nicolet, B.H. *et al*, *J. Am. Chem. Soc.*, 1927, **49**, 2066 (*synth*)
U.S. Pat., 4 247 468, (1981); *CA*, **94**, 174376h.
Ikuta, H. *et al*, *J. Med. Chem.*, 1987, **30**, 1995 (*chloride, amide, pmr*)

2,10-Dibromo-3-chloro-7-chamigren-9-ol D-80081

[73494-22-1]

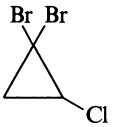


$C_{15}H_{23}Br_2ClO$ M 414.607

Metab. of *Laurencia nipponica*. Cryst. (diisopropyl ether). Mp 119-120°. $[\alpha]_D^{19}$ +25.3° (c, 1.39 in $CHCl_3$).

Suzuki, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3371.

1,1-Dibromo-2-chlorocyclopropane D-80082



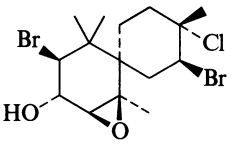
$C_3H_3Br_2Cl$ M 234.317

(±)-***form*** [77628-95-6]

$Bp_{0.001}$ 80°.

Weber, A. *et al*, *Helv. Chim. Acta*, 1988, **71**, 2026 (*synth, ir, pmr, ms*)

4,10-Dibromo-3-chloro-7,8-epoxy-9-hydroxy-α-chamigrane D-80083



$C_{15}H_{23}Br_2ClO_2$ M 430.606

Constit. of *Laurencia glomerata*. Gum. $[\alpha]_D^{25}$ +32.7° (c, 0.91 in $CHCl_3$).

Elsworth, J.F. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 893 (*isol, pmr, cmr*)

1,1-Dibromo-1-chloro-2,2,2-trifluoroethane, 9CI D-80084

[754-17-6]

F_3CCBr_2Cl

$C_2Br_2ClF_3$ M 276.278

Shows fire-extinguishing props. Mp 42-45°. Bp 92-95°.

▷ Irritant.

[29256-79-9]

Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1970, **35**, 1302 (*synth*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Okuhara, K., *J. Org. Chem.*, 1978, **43**, 2745 (*synth, F-19 nmr*)

1,2-Dibromo-1-chloro-1,2,2-trifluoroethane, 9CI D-80085

2-Chloro-1,2-dibromo-1,1,2-trifluoroethane. Freon 113B2

[354-51-8]

$F_2CBrCBrClF$

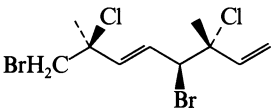
$C_2Br_2ClF_3$ M 276.278

Refrigerant (CFC). Aerosol propellant. d_4^{20} 2.248. Mp −72.8°. Bp 93-94°. n_D^{20} 1.427.

Glockler, G. *et al*, *J. Chem. Phys.*, 1941, **9**, 387 (*raman*)
Drysdale, J.J. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 319 (*synth*, *F*-19 *nmr*)
Dean, R.R. *et al*, *Trans. Faraday Soc.*, 1968, **64**, 1409 (*pmr*, *F*-19 *nmr*)
Norris, R.D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 182 (*F*-19 *nmr*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Majer, V. *et al*, *Collect. Czech. Chem. Commun.*, 1981, **46**, 817 (*props*)
Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co. Ltd, 1988, 084 (*F*-19 *nmr*)

4,8-Dibromo-3,7-dichloro-3,7-dimethyl-1,5-octadiene D-80086

[119903-44-5]

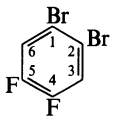


$C_{10}H_{14}Br_2Cl_2$ M 364.934
Constit. of *Plocamium hamatum*. Oil. $[\alpha]_D$ −7° (c, 0.006 in $CHCl_3$).

Coll, J.C. *et al*, *Aust. J. Chem.*, 1988, **41**, 1743.

1,2-Dibromo-4,5-difluorobenzene, 9CI D-80087

[64695-78-9]



$C_6H_2Br_2F_2$ M 271.887
Cryst. (Et_2O). Mp 32.5-33.5°. Readily subl.

[101051-60-9]

Cervena, I. *et al*, *Collect. Czech. Chem. Commun.*, 1977, **42**, 2001 (*synth*)

1,4-Dibromo-2,5-difluorobenzene, 9CI D-80088

[327-51-5]

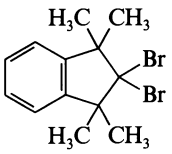
$C_6H_2Br_2F_2$ M 271.887
Cryst. (EtOH). Mp 64.5-65.5°. Bp_{20} 96°. Subl. slowly on standing.

Finger, G.C. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 145 (*synth*)
Gatowsky, H.S. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 4809 (*F*-19 *nmr*)
Wasylishen, R. *et al*, *Can. J. Chem.*, 1970, **48**, 2885 (*pmr*)
Anderson, J.M. *et al*, *J. Magn. Reson.*, 1981, **44**, 1 (*pmr*)

2,2-Dibromo-2,3-dihydro-1,1,3,3-tetramethyl-1*H*-indene, 9CI D-80089

2,2-Dibromo-1,1,3,3-tetramethylindane

[118617-97-3]

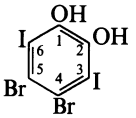


$C_{13}H_{16}Br_2$ M 332.077
Cryst. Mp 43-44°.

Guziec, F.S. *et al*, *Synthesis*, 1988, 547 (*synth*, *ir*, *pmr*, *cmr*)

4,5-Dibromo-3,6-diiodo-1,2-benzenediol, 9CI D-80090

4,5-Dibromo-3,6-diiodocatechol

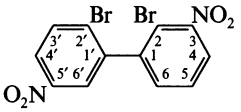


$C_6H_2Br_2I_2O_2$ M 519.698
Di-Me ether: [120231-43-8]. *1,2-Dibromo-3,6-diiodo-4,5-dimethoxybenzene. 4,5-Dibromo-3,6-diiodoveratrole*
$C_8H_6Br_2I_2O_2$ M 547.751
Needles ($CHCl_3$/MeOH). Mp 144-145°.

Meador, M.A. *et al*, *J. Org. Chem.*, 1989, **54**, 2336 (*synth*, *ms*)

2,2′-Dibromo-3,5′-dinitrobiphenyl D-80091

[87682-47-1]



$C_{12}H_6Br_2N_2O_4$ M 401.998
Yellow prisms (MeOH). Mp 124-125°.

Baker, W. *et al*, *J. Chem. Soc.*, 1960, 414 (*synth*)
Dougherty, T.K. *et al*, *J. Org. Chem.*, 1983, **48**, 5273 (*synth*)

2,2′-Dibromo-5,5′-dinitrobiphenyl D-80092

[52026-22-9]

$C_{12}H_6Br_2N_2O_4$ M 401.998
Pale-yellow prisms ($EtOH/Me_2CO$). Mp 220-221°.

Baker, W. *et al*, *J. Chem. Soc.*, 1960, 414 (*synth*)
Dougherty, T.K. *et al*, *J. Org. Chem.*, 1983, **48**, 5273 (*synth*, *ir*, *pmr*)

5,5′-Dibromo-2,2′-dinitrobiphenyl D-80093

$C_{12}H_6Br_2N_2O_4$ M 401.998
Yellow prisms (EtOAc). Mp 204-205°.

Murakami, M. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1949, **70**, 236 (*synth*)
Forrest, J., *J. Chem. Soc.*, 1960, 594.

1,3-Dibromo-1,1,2,2,3,3-hexafluoropropane, 9CI D-80094

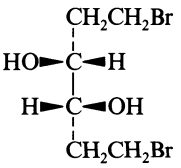
[4259-29-4]

$F_2CBrCF_2CF_2Br$

$C_3Br_2F_6$ M 309.831
Liq. d_4^{20} 2.172. Bp 74.2°. n_D^{20} 1.3590, $n_D^{30.2}$ 1.3526.

Hauptschein, M. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 848 (*synth*)
Nodiff, E.A. *et al*, *J. Org. Chem.*, 1953, **18**, 235 (*props*)

1,6-Dibromo-3,4-hexanediol, 9CI D-80095



(3*R*,4*R*)-*form*

$C_6H_{12}Br_2O_2$ M 275.968
(3R,4R)-form [82188-39-4]

Mp 90-91°. $[\alpha]_D^{27}$ +58.4° (c, 2.16 in $CHCl_3$).
Bis-4-methylbenzenesulfonyl: Plates (EtOH aq.). Mp 139.5-141°. $[\alpha]_D^{25}$ +74.3° (c, 3.2 in $CHCl_3$).
[53399-76-1]
Cope, A.C. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 5916 (*synth*)
Cerè, V. *et al*, *J. Org. Chem.*, 1988, **53**, 5689 (*synth, cmr*)

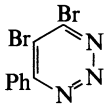
4,5-Dibromo-6-methyl-1,2,3-triazine D-80096

[114078-91-0]

$C_4H_3Br_2N_3$ M 252.896
Granules (hexane/Et_2O). Mp 130-132° dec.
Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

4,5-Dibromo-6-phenyl-1,2,3-triazine D-80097

[114078-93-2]



$C_9H_5Br_2N_3$ M 314.967
Needles (hexane/Et_2O). Mp 110-112° dec.
Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

4,9-Dibromopyrene D-80098

$C_{16}H_8Br_2$ M 360.047
Cryst. ($CHCl_3$). Mp 247°.
Blatter, K. *et al*, *Synthesis*, 1989, 356 (*synth, ir, pmr, cmr, ms*)

2,6-Dibromo-4(1*H*)-pyridone D-80099

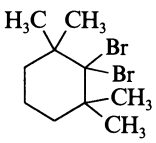
2,6-Dibromo-4-hydroxypyridine
$C_5H_5Br_2NO$ M 254.909
Me ether: [117873-72-0]. *2,6-Dibromo-4-methoxypyridine*
$C_6H_5Br_2NO$ M 266.920
Needles. Mp 136°.
Den Hertog, H.J., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1948, **67**, 381.
Neumann, U. *et al*, *Chem. Ber.*, 1989, **122**, 589.

4,6-Dibromo-2(1*H*)pyridone D-80100

2,4-Dibromo-6-hydroxypyridine
$C_5H_3Br_2NO$ M 252.893
Me ether: [117873-73-1]. *2,4-Dibromo-6-methoxypyridine*
$C_6H_5Br_2NO$ M 266.920
Cryst. Mp 92°.
Neumann, U. *et al*, *Chem. Ber.*, 1989, **122**, 589.

2,2-Dibromo-1,1,3,3-tetramethylcyclohexane, 9CI D-80101

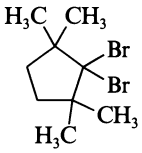
[118617-98-4]



$C_{10}H_{18}Br_2$ M 298.060
Cryst. Mp 185°.
Guziec, F.S. *et al*, *Synthesis*, 1988, 547 (*synth, ir, pmr, cmr*)

2,2-Dibromo-1,1,3,3-tetramethylcyclopentane, 9CI D-80102

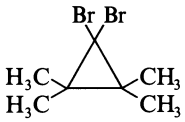
[118617-99-5]



$C_9H_{16}Br_2$ M 284.033
Cryst. Mp 159-161°. Unstable, must be kept in dark and cold.
Guziec, F.S. *et al*, *Synthesis*, 1988, 547 (*synth, ir, pmr, cmr*)

1,1-Dibromo-2,2,3,3-tetramethylcyclopropane, 9CI D-80103

[22715-57-7]



$C_7H_{12}Br_2$ M 255.980
Plates (EtOH aq.). Mp 78-80°.
Hackett, M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1449 (*synth, pmr*)

3,3-Dibromo-2,2,4,4-tetramethylpentane, 9CI D-80104

*Dibromodi-*tert*-butylmethane*
[84679-81-2]

$[(H_3C)_3C]_2CBr_2$

$C_9H_{18}Br_2$ M 286.049
Cryst. by subl. Mp 183-184° (175°).
Kalinowski, H. *et al*, *Org. Magn. Reson.*, 1983, **21**, 64 (*synth, cmr, pmr*)
Guziec, F.S. *et al*, *Synthesis*, 1988, 547 (*synth*)

4,5-Dibromo-1,2,3-triazine D-80105

[114078-89-6]

$C_3HBr_2N_3$ M 238.869
Needles (hexane/Et_2O). Mp 138-139° dec.
Ohsawa, A. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3838 (*synth, pmr*)

2,2-Dibromo-1,1,1-trifluoroethane, 9CI D-80106

[354-30-3]

F_3CCHBr_2

$C_2HBr_2F_3$ M 241.833
Shows anaesthetic activity, component of fire extinguishers. d_4^{24} 2.22. Bp 73°. n_D^{26} 1.4029.
[108662-84-6]
Robbins, B.H., *J. Pharmacol.*, 1946, **86**, 197 (*use*)

McBee, E.T. *et al*, *Ind. Eng. Chem.*, 1947, **39**, 420 (*synth*)
Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co Ltd, Japan, 1980, 030, 031 (*F*-19 *nmr*, *pmr*)

1,11-Dibromo-6-undecanone, 9CI D-80107

[116288-13-2]

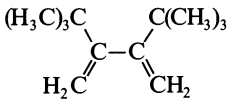
$BrCH_2(CH_2)_4CO(CH_2)_4CH_2Br$

$C_{11}H_{20}Br_2O$ M 328.086
Oil. Bp_2 153°.

Momenteau, M. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1988, 283 (*synth*, *pmr*)

2,3-Di-*tert*-butyl-1,3-butadiene D-80108

Updated Entry replacing D-02189
2,2,5,5-Tetramethyl-3,4-bis(methylene)hexane, *9CI*
[3378-20-9]

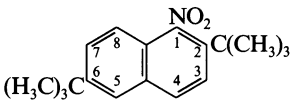


$C_{12}H_{22}$ M 166.306
Liq. Bp_{12} 58°.

Lenoir, D., *Chem. Ber.*, 1978, **111**, 411 (*synth*, *ir*, *pmr*)
Roth, W.R. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1883 (*props*)

2,6-Di-*tert*-butyl-1-nitronaphthalene D-80109

2,6-Bis(1,1-dimethylethyl)-1-nitronaphthalene
[20870-30-8]



$C_{18}H_{23}NO_3$ M 301.385
Light yellow needles (EtOH). Mp 80-81°. Light-sensitive.

Döpp, D. *et al*, *Chem. Ber.*, 1988, **121**, 2045 (*synth*, *pmr*, *cmr*, *uv*, *ms*)

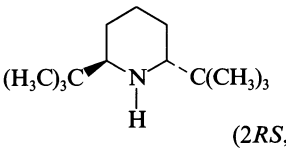
3,7-Di-*tert*-butyl-1-nitronaphthalene D-80110

3,7-Bis(1,1-dimethylethyl)-1-nitronaphthalene
[20820-31-9]
$C_{18}H_{23}NO_2$ M 285.385
Yellow needles (EtOH). Mp 64-65°. Light-sensitive.

Döpp, D. *et al*, *Chem. Ber.*, 1988, **121**, 2045 (*synth*, *pmr*, *cmr*, *uv*, *ms*)

2,6-Di-*tert*-butylpiperidine D-80111

2,6-Bis(1,1-dimethylethyl)piperidine, *9CI*



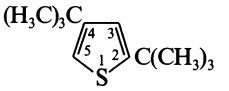
(2*RS*,6*RS*)-*form*

$C_{13}H_{27}N$ M 197.363
(*2RS,6RS*)-*form* [101166-52-3]
(±)-trans-form
Picrate: Mp 165.5-166°.
(*2RS,6SR*)-*form* [66922-18-7]
cis-form
Bp_{10} 95-97°.
Picrate: Mp 224-225°.

Day, J.C., *J. Org. Chem.*, 1978, **43**, 3646 (*synth*, *pmr*, *cmr*, *N*-15 *nmr*)
Francis, R.F. *et al*, *J. Org. Chem.*, 1986, **51**, 1889 (*synth*, *pmr*, *cmr*)

2,4-Di-*tert*-butylthiophene D-80112

2,4-Bis(1,1-dimethylethyl)thiophene, *9CI*
[33369-81-2]



$C_{12}H_{20}S$ M 196.356
Mp −1°. Bp_{752} 220.4°.

Wynberg, H. *et al*, *J. Org. Chem.*, 1965, **30**, 1058 (*synth*, *uv*, *ir*, *pmr*)
Nakayama, J. *et al*, *Tetrahedron Lett.*, 1988, **29**, 1161 (*synth*)

3,4-Di-*tert*-butylthiophene D-80113

Updated Entry replacing D-02263
3,4-Bis(1,1-dimethylethyl)thiophene, *9CI*
[22808-03-3]
$C_{12}H_{20}S$ M 196.356
Mp 43-43.5°. Bp_4 75° (bulb) . Highly strained.
1,1-Dioxide: [116375-45-2].
$C_{12}H_{20}O_2S$ M 228.355
Cryst. Mp 132.5-133°.

Brandsma, L. *et al*, *J. Chem. Soc.*, *Chem. Commun.*, 1980, 922 (*synth*, *cryst struct*, *pmr*)
Nakayama, J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6598 (*use*)
Nakayama, J. *et al*, *Tetrahedron Lett.*, 1988, **29**, 1161 (*dioxide*)

Dicarbon dioxide D-80114

Ethenedione, *9CI*
[4363-38-6]

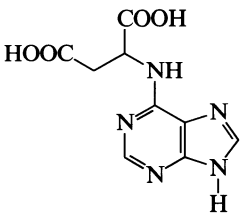
OC=CO

C_2O_2 M 56.021
Not known. Calcns. suggest extreme instability.

Hoffman, R.W. *et al*, *Tetrahedron*, 1965, **21**, 891.
Herberhold, M. *et al*, *Z. Naturforsch.*, *B*, 1976, **31**, 35.

6-(1,2-Dicarboxyethylamino)purine D-80115

N-*1H-Purin-6-ylaspartic acid*, *9CI*
[26511-42-2]



$C_9H_9N_5O_4$ M 251.201
Isol. from *Fusarium* sp.
[26287-66-1]

Ballio, A. *et al*, *Gazz. Chim. Ital.*, 1964, **94**, 156 (*isol*)
McCloskey, J.A. *et al*, *Biomed. Mass Spectrom.*, 1975, **2**, 90 (*ms*)

1,1-Dichloroethylene, 8CI D-80116

1,1-Dichloroethene, 9CI. Vinylidene chloride

[75-35-4]

$H_2C{=}CCl_2$

$C_2H_2Cl_2$ M 96.943

Intermediate in production of plastics as comonomer with vinyl chloride, acrylonitrile, acrylates etc. Reacts with alcohols and halides to give carboxylic acids. Volatile liq. d^{20} 1.218. Fp −122.5°. Bp 31.7°, Bp °(37°) . n_D^{20} 1.4249. Readily polymerises.

▷ Mod. toxic by inhalation, TLV 40. Exp. carcinogen. Extremely flammable. Rapidly absorbs O_2 forming violently explosive peroxide. KV9275000.

Kunichika, S. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1950, **53**, 407; *CA*, **47**, 5871 (*synth*)
Miyajima, G. *et al*, *J. Phys. Chem.*, 1971, **75**, 331 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 118.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 354.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 1088.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 279.

1,1-Dichloro-1-fluoroethane, 9CI D-80117

1-Fluoro-1,1-dichloroethane. HCFC 141B

[1717-00-6]

H_3CCCl_2F

$C_2H_3Cl_2F$ M 116.950

Alternative refrigerant. Shows anaesthetic props. d_4^{10} 1.250. Fp −103.5°. Bp 32°. n_D^{10} 1.360.

Brown, J.H. *et al*, *J. Soc. Chem. Ind., London*, 1948, **67**, 331 (*synth*)
Smith, D.C. *et al*, *J. Chem. Phys.*, 1952, **20**, 473 (*ir, raman*)
Durig, J.R. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 175 (*ir, raman*)

1,1-Dichloro-2-fluoroethene, 9CI D-80118

[359-02-4]

$Cl_2C{=}CHF$

C_2HCl_2F M 114.934

d_4^{20} 1.383. Mp −108.8°. Bp 37-39°. n_D^{20} 1.4036.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 402 (*synth*)
Yanwood, J., *J. Chem. Soc.*, 1965, 7481 (*ir, raman*)
Craig, N.C., *J. Mol. Spectrosc.*, 1967, **23**, 307 (*ir, raman*)
Moehlmann, J.G. *et al*, *J. Chem. Phys.*, 1975, **62**, 3052 (*synth, ir*)

2,2-Dichloro-6-heptenoic acid, 9CI D-80119

[105764-09-8]

$H_2C{=}CH(CH_2)_3CCl_2COOH$

$C_7H_{10}Cl_2O_2$ M 197.060

$Bp_{<0.1}$ 60-65° (bulb) .

Et ester: [105764-08-7].
$C_9H_{14}Cl_2O_2$ M 225.114
Liq. $Bp_{0.5}$ 80-85°.

Hayes, T.K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5533 (*synth, pmr, ir, ms, cmr*)

1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane, 9CI D-80120

[661-97-2]

$F_3CCClFCClF_2$

$C_3Cl_2F_6$ M 220.929

Refrigerant. Solv. in the manuf. of polyethers and for disperse dyes. d_4^{20} 1.590, d_4^{20} 1.598. Fp −136° (−131.1°). Bp 34.5°. n_D^{20} 1.3029, n_D^{0} 1.3110.

Park, J.D. *et al*, *J. Org. Chem.*, 1961, **26**, 4017 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*synth, props*)
Schmeisser, M. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1967, **6**, 627 (*synth*)
De Marco, A. *et al*, *J. Magn. Reson.*, 1972, **6**, 208 (*F nmr*)
Capriel, P. *et al*, *Tetrahedron*, 1979, **35**, 2661 (*F nmr*)

1,3-Dichloro-1,1,2,2,3,3-hexafluoropropane, 9CI D-80121

Freon 216

[662-01-1]

$F_2CClCF_2CClF_2$

$C_3Cl_2F_6$ M 220.929

Refrigerant, working fluid for rankine cycle electric power systems, shows anaesthetic props. d_4^{20} 1.573. Fp −125.3° (−193.7°). Bp 33.8° (36.1°) . $n_D^{22.2}$ 1.3022, n_D^{20} 1.3030.

Hauptschein, M. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 848 (*synth*)
Nodiff, E.A. *et al*, *J. Org. Chem.*, 1953, **18**, 235 (*props*)
Angell, C.L., *J. Chem. Eng. Data*, 1964, **9**, 341 (*ir, raman*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
White, H.F., *Anal. Chem.*, 1966, **38**, 625 (*F nmr*)
Schmeisser, M. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1967, **6**, 627 (*synth*)
Fernholt, L. *et al*, *Acta Chem. Scand., Ser. A*, 1978, **32**, 225 (*ed*)

2,2-Dichloro-1,1,1,3,3,3-hexafluoropropane, 9CI D-80122

[1652-80-8]

$F_3CCCl_2CF_3$

$C_3Cl_2F_6$ M 220.929

Solv. for disperse dyes. Shows anaesthetic props. Mp 3° (−10 to −13°). Bp 32.5-33°. n_D^{20} 1.3050 (1.3032).

Maynard, J.T., *J. Org. Chem.*, 1963, **28**, 112 (*synth, ir*)
Farah, B.S. *et al*, *J. Org. Chem.*, 1965, **30**, 1241 (*synth*)
Weigert, F.J. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5314 (*F nmr*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Buerger, H. *et al*, *Spectrochim. Acta, Part A*, 1979, **35**, 525 (*ir, raman*)
Eujen, R. *et al*, *J. Fluorine Chem.*, 1983, **22**, 263 (*F nmr*)

2,2-Dichloro-7-octenoic acid D-80123

[105764-15-6]

$H_2C{=}CH(CH_2)_4CCl_2COOH$

$C_8H_{12}Cl_2O_2$ M 211.087

$Bp_{<0.1}$ 90-95° (bulb) .

Et ester: [105764-14-5].
$C_{10}H_{16}Cl_2O_2$ M 239.141
$Bp_{<0.1}$ 84-88°.

Amide: [115119-89-6].
$C_8H_{13}Cl_2NO$ M 210.102
Pale yellow solid.

Nitrile: [115119-91-0].
$C_8H_{11}Cl_2N$ M 192.087

Oil.

Hayes, T.K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5533 (*synth, derivs, pmr, ir, ms, cmr*)

1,5-Dichloro-3-pentanol D-80124

[72548-31-3]

$ClCH_2CH_2CH(OH)CH_2CH_2Cl$

$C_5H_{10}Cl_2O$ M 157.039
Oil. $Bp_{0.1}$ 64-70°.

Reese, C.B. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2881 (*synth, pmr, cmr*)

1,5-Dichloro-3-pentanone, 9CI D-80125

Di(2-chloroethyl) ketone. 2,2'-Dichlorodiethyl ketone

[3592-25-4]

$ClCH_2CH_2COCH_2CH_2Cl$

$C_5H_8Cl_2O$ M 155.023
Liq. $Bp_{0.8}$ 78°. Stable at 0°, polym. at r.t.

Cardwell, H.M.E. *et al*, *J. Chem. Soc.*, 1949, 708 (*synth*)
Bowden, K. *et al*, *J. Chem. Soc.*, 1952, 1164 (*synth*)
Arbuzov, Y.A. *et al*, *Zh. Obshch. Khim.*, 1962, **32**, 3681; (*synth*)
Owen, G.R. *et al*, *J. Chem. Soc. C*, 1970, 2401 (*synth, ir, pmr, ms*)

2,5-Dichloro-1-pentene D-80126

[58568-26-6]

$H_2C{=}CClCH_2CH_2CH_2Cl$

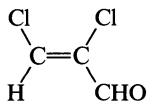
$C_5H_8Cl_2$ M 139.024
Oil. Bp_{20} 58-60°.

Wender, P.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2218 (*synth, pmr, ir, ms*)

2,3-Dichloro-2-propenal D-80127

α,β-Dichloroacrolein

[26910-68-9]



$C_3H_2Cl_2O$ M 124.954

(Z)-form [6695-22-3]
d_4^{20} 1.390. Bp_9 44°. n_D^{25} 1.5110. The *E*-form could not be obt.

2,4-Dinitrophenylhydrazone: Deep red cryst. (EtOH). Mp 244° dec. (235°).

[99414-75-2, 99569-10-5]

Tobey, W. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 2478 (*synth, ir, pmr*)
Annenkova, V. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1970, 223 (*synth*)
Wille, F. *et al*, *Z. Naturforsch., B*, 1977, 733 (*synth, pmr*)
Roedig, A. *et al*, *Justus Liebigs Ann. Chem.*, 1979, 194 (*synth, ir, pmr, config*)
Rosen, J.D. *et al*, *Mutat. Res.*, 1980, **78**, 113 (*synth, pmr, ms*)
Ruzo, L.O. *et al*, *J. Agric. Food Chem.*, 1985, **33**, 272 (*pmr*)
Segall, Y. *et al*, *Mutat. Res.*, 1985, **158**, 61 (*tox*)
Bostroem, G.O. *et al*, *J. Mol. Struct.*, 1988, **172**, 227 (*struct*)

3,3-Dichloro-2-propenal, 9CI D-80128

β,β-Dichloroacrolein

$Cl_2C{=}CHCHO$

$C_3H_2Cl_2O$ M 124.954

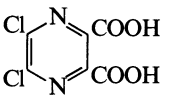
Pale yellow liq. Sol. H_2O. Bp 124°, Bp_{21} 38-39°. n_D^{24} 1.5062.
▷ Lachrymator.

2,4-Dinitrophenylhydrazone: Mp 164-165°.

Kharasch, M.S. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 1105 (*synth, deriv*)
Soulen, R.L. *et al*, *J. Org. Chem.*, 1971, **36**, 3386 (*synth*)
Pochat, F. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 3145 (*ir*)
Ellern, J.B. *et al*, *J. Org. Chem.*, 1972, **37**, 4485 (*synth, deriv, ir*)
Coleman, W.E. *et al*, *Environ. Sci. Technol.*, 1984, **18**, 674 (*glc, ms*)
Hanack, M. *et al*, *Synthesis*, 1987, 944 (*synth*)

5,6-Dichloro-2,3-pyrazinedicarboxylic acid D-80129

[59715-45-6]



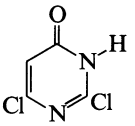
$C_6H_2Cl_2N_2O_4$ M 236.998

Dinitrile: [56413-95-7]. *2,3-Dichloro-5,6-dicyanopyrazine*
$C_6Cl_2N_4$ M 198.998
Readily accessible intermed. for polycyclic heteroaromatics. Needles ($CHCl_3$). Mp 179-180°.

Suzuki, T. *et al*, *J. Heterocycl. Chem.*, 1986, **23**, 1419.
Ried, W. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 1197 (*use*)

2,6-Dichloro-4(*3H*)-pyrimidinone D-80130

[120977-94-8]



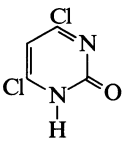
$C_4H_2Cl_2N_2O$ M 164.978
Cryst. (H_2O). Mp 170-171°. Reg. no. refers to the (prob. unfavoured) 1*H*-form.

Hübsch, W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 738.

4,6-Dichloro-2(*1H*)-pyrimidinone D-80131

4,6-Dichloro-2-hydroxypyrimidine

[6297-80-9]

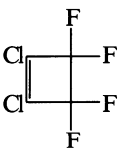


$C_4H_2Cl_2N_2O$ M 164.978
Cryst. powder. Mp 157°. Higher Mps previously reported are said to indicate a high content of the Na salt.

Hübsch, W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 738.

1,2-Dichloro-3,3,4,4-tetrafluorocyclobutene, 9CI D-80132

[377-93-5]



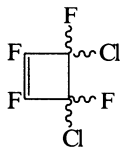
$C_4Cl_2F_4$ M 194.943
d_4^{25} 1.534. Mp −43.4° (−48°). Bp 67.1°. n_D^{25} 1.3699.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 281 (*synth, props*)

Harris, R.K. *et al*, *J. Magn. Reson.*, 1969, **1**, 362 (*F*-19 *nmr*)
King, B.R. *et al*, *J. Fluorine Chem.*, 1972, **1**, 283 (*synth*)
Chia, L.S. *et al*, *Can. J. Chem.*, 1974, **52**, 3484 (*Cl-nqr*)
Bauer, G. *et al*, *Z. Naturforsch.*, *B*, 1979, **34**, 1249 (*synth*)

3,4-Dichloro-1,2,3,4-tetrafluorocyclobutene, 9CI — D-80133

[425-62-7]



$C_4Cl_2F_4$ M 194.943
Bp 65.5°. n_D^{20} 1.375. No stereoisomers reported.

Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1955, 3880 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864.

1,1-Dichloro-1,2,2,2-tetrafluoroethane — D-80134

[374-07-2]

F_3CCFCl_2

$C_2Cl_2F_4$ M 170.921
Refrigerant component. d_4^{25} 1.455. Fp −56.6°, Mp −94°. Bp 3-4°. n_D^0 1.3092.

▷ Irritant.

[1320-37-2]

Nielsen, J.R. *et al*, *J. Chem. Phys.*, 1953, **21**, 383 (*ir*, *raman*)
Goldwhite, H. *et al*, *J. Chem. Soc.*, 1961, 3825 (*synth*, *ir*)
Vecchio, M. *et al*, *J. Fluorine Chem.*, 1974, **4**, 117 (*synth*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Eujen, R. *et al*, *J. Fluorine Chem.*, 1983, **22**, 263 (*F*-19 *nmr*)

1,1-Dichloro-2,3,3,3-tetrafluoro-1-propene, 9CI — D-80135

[2804-55-9]

$Cl_2C{=}CFCF_3$

$C_3Cl_2F_4$ M 182.932
Fumigant. d_4^{20} 1.539. Fp −139.6°. Bp 45-46.5° (43.5°) . n_D^{20} 1.3504.

[111548-56-2]

Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 2257 (*synth*)
Paleta, O. *et al*, *Bull. Soc. Chim. Fr.*, 1986, 920 (*synth*, *F nmr*)

1,2-Dichloro-1,3,3,3-tetrafluoro-1-propene, 9CI — D-80136

[431-53-8]

$F_3CCCl{=}CFCl$

$C_3Cl_2F_4$ M 182.932
Fumigant. Fp −137°. Bp 47.3°. Bp refers to mixt. of stereoisomers.

[73562-83-1, 73562-84-2, 111548-56-2]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1946, **68**, 496 (*synth*)
McConnell, H.M. *et al*, *J. Chem. Phys.*, 1956, **25**, 184 (*F nmr*)
Swalden, J.D. *et al*, *J. Chem. Phys.*, 1961, **34**, 2122 (*F nmr*)

3,3-Dichloro-2,2,4,4-tetramethylpentane, 9CI — D-80137

Di-tert-*butyldichloromethane*

[79991-69-8]

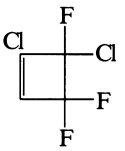
$[(H_3C)_3C]_2CCl_2$

$C_9H_{18}Cl_2$ M 161.694
Cryst. by subl. Mp 103-104°.

Kalinowski, H. *et al*, *Org. Magn. Reson.*, 1983, **21**, 64 (*synth*, *cmr*, *pmr*)

1,4-Dichloro-3,3,4-trifluorocyclobutene, 9CI — D-80138

[2927-72-2]



$C_4HCl_2F_3$ M 176.953
Bp 91-92°. n_D^{25} 1.3942.

Raasch, M.S. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 2678 (*synth*)
Park, J.D. *et al*, *J. Org. Chem.*, 1965, **30**, 400 (*synth*, *ir*, *F*-19 *nmr*)
Newmark, R.A. *et al*, *J. Magn. Reson.*, 1969, **1**, 418 (*F*-19 *nmr*)

1,1-Dichloro-1,2,2-trifluoroethane, 9CI — D-80139

[812-04-4]

Cl_2CFCF_2H

$C_2HCl_2F_3$ M 152.931
Bp 59-61°, Bp 30.2°.

Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1960, 4503 (*synth*)
Fuller, G. *et al*, *Tetrahedron*, 1962, **18**, 123 (*synth*)

1,2-Dichloro-1,1,2-trifluoroethane, 9CI — D-80140

[354-23-4]

$F_2CClCHClF$

$C_2HCl_2F_3$ M 152.931
Refrigerant. Shows anaesthetic properties. Gas. $d_4^{27.4}$ 1.498. Bp 28-30°. n_D^{15} 1.3371.

▷ Irritant, convulsant.

[34077-87-7, 90454-18-5]

Glockler, G. *et al*, *J. Chem. Phys.*, 1941, **9**, 387 (*raman*)
Park, J.D. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 711 (*synth*, *ir*)
Fuller, G. *et al*, *Tetrahedron*, 1962, **18**, 123 (*tox*)
Doucet, J. *et al*, *J. Chem. Phys.*, 1975, **62**, 355 (*uv*, *pe*)
Kirk-Othmer Encycl. Chem. Technol., 3*rd Ed.*, 1978-1984, *Wiley*, *NY*, 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 861 (*props*)
Capnel, P. *et al*, *Tetrahedron*, 1979, **35**, 2661 (*F*-19 *nmr*)
Service, C.F. *et al*, *J. Fluorine Chem.*, 1982, **20**, 135 (*synth*)

2,2-Dichloro-1,1,1-trifluoroethane, 9CI — D-80141

HCFC 123. Freon 123

[306-83-2]

F_3CCHCl_2

$C_2HCl_2F_3$ M 152.931
Used in aerosol formulations, refrigerant, degreasing solvent. Shows anaesthetic props. Gas. d_4^{15} 1.475. Mp −107°. Bp 28.7°, Bp_{747} 27.1°. n_D^{15} 1.333.

McBee, E.T. *et al*, *Ind. Eng. Chem.*, 1947, **39**, 409 (*synth*)
Nielsen, J.R. *et al*, *J. Chem. Phys.*, 1953, **21**, 1060 (*ir*, *raman*)

Ng, S., *J. Magn. Reson.*, 1972, **7**, 370 (*pmr*)
Burns, T.H.S. *et al*, *Anaesthesia*, 1982, **37**, 278 (*use*)
Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co., 1988, 016, 017 (*F-19 nmr, pmr*)

1,1-Dichloro-1,2,2-trifluoro-2-iodoethane, 9CI D-80142

[661-66-5]

ICF_2CCl_2F

$C_2Cl_2F_3I$ M 278.827
Light-sensitive liq. d_4^{25} 2.189. Bp 103.1°. n_D^{25} 1.444.
▷ Lachrymator.

Chambers, R.D. *et al*, *J. Chem. Soc.*, 1961, 3779 (*ir*)
Bissell, E.R. *et al*, *J. Org. Chem.*, 1962, **27**, 1482 (*synth*)
Dean, R.R. *et al*, *Trans. Faraday Soc.*, 1968, **64**, 1409 (*F-nmr*)

1,2-Dichloro-1,1,2-trifluoro-2-iodoethane, 9CI D-80143

[354-61-0]

$F_2CClCClFI$

$C_2Cl_2F_3I$ M 278.827
Liq. d_4^{25} 2.199. Bp 103.9°, Bp_{100} 43-44°. $n_D^{25.2}$ 1.448. Turns pink in light.

[57171-62-7]

Hazeldine, R.N., *J. Chem. Soc.*, 1953, 1764 (*uv*)
Hauptschein, M. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2495 (*synth, ir*)
Bissell, E.R. *et al*, *J. Org. Chem.*, 1962, **27**, 1482 (*synth*)
Capnel, P. *et al*, *Tetrahedron*, 1979, **35**, 2661 (*F-19 nmr*)

2,2-Dichloro-1,1,1-trifluoropropane, 9CI D-80144

[7126-01-4]

$F_3CCCl_2CH_3$

$C_3H_3Cl_2F_3$ M 166.957
Shows anaesthetic props. d_4^{20} 1.3842. Mp 13.8°. Bp 48.8°. n_D^{20} 1.348.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 1157 (*synth*)
McBee, E.T. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 944 (*synth*)

2,3-Dichloro-1,1,1-trifluoropropane, 9CI D-80145

[338-75-0]

$F_3CCHClCH_2Cl$

$C_3H_3Cl_2F_3$ M 166.957
Shows anaesthetic props. Bp 76-77°. n_D^{20} 1.3671.

Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1953, 1199, 3371 (*synth, ir*)
Di Paolo, T. *et al*, *J. Pharm. Sci.*, 1979, **68**, 39 (*pharmacol*)

3,3-Dichloro-1,1,1-trifluoropropane, 9CI D-80146

[460-69-5]

$F_3CCH_2CHCl_2$

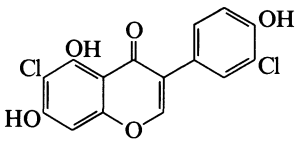
$C_3H_3Cl_2F_3$ M 166.957
Shows anaesthetic props. d_4^{20} 1.4408. Bp 72-74°. n_D^{20} 1.3531.

McBee, E.T. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 944 (*synth*)
Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1953, 1199 (*synth, ir*)
Varushchenko, R.M. *et al*, *Russ. J. Phys. Chem.*, 1972, **46**, 755 (*props*)
Di Paolo, T. *et al*, *J. Pharm. Sci.*, 1979, **68**, 39 (*pharmacol*)

3′,6-Dichloro-4′,5,7-trihydroxyisoflavone D-80147

*6-Chloro-3-(3-chloro-4-hydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one. 3′,6-Dichlorogenistein*

[64545-65-9]

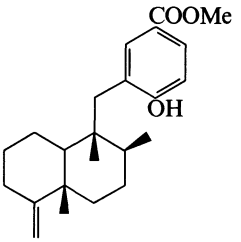


$C_{15}H_8Cl_2O_5$ M 339.131
Metab. of *Streptomyces griseus*. All isolations of isoflavonoids from microorganisms are considered dubious. Prob. artifact derived from the soybean medium.

König, W.A. *et al*, *Helv. Chim. Acta*, 1977, **60**, 2071 (*isol, ir, pmr, ms, struct*)

Dictyoceratin D-80148

[123062-43-1]



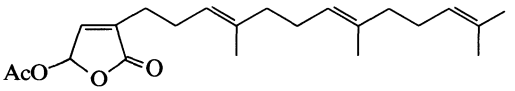
$C_{23}H_{32}O_3$ M 356.504
Metab. of *Dactylospongia* sp. Solid.

Kushlan, D.M. *et al*, *Tetrahedron*, 1989, **45**, 3307.

Dictyodendrillolide D-80149

*5-(Acetyloxy)-3-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2(5*H*)-furanone, 9CI*

[117585-47-4]



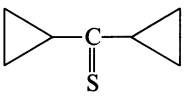
$C_{22}H_{32}O_4$ M 360.492
Constit. of a *Dictyodendrilla* sp. Oil. $[\alpha]_D^{23}$ +21.9° (c, 0.43 in $CHCl_3$).

Cambie, R.C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1014.

Dicyclopropylmethanethione, 9CI D-80150

Dicyclopropyl thioketone

[38381-24-7]

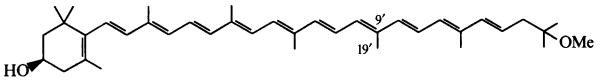


$C_7H_{10}S$ M 126.222
Orange liq.

Fournier, C. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2753; 1980, 463 (*synth, uv, pmr*)
Andrieu, C.G. *et al*, *Org. Magn. Reson.*, 1978, **11**, 528 (*cmr*)
Mieloszynski, J.L. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1985, **104**, 9 (*cmr*)

3′,4′-Didehydro-1′,2′-dihydro-1′-methoxy-β,ψ-caroten-3-ol D-80151

[119188-86-2]



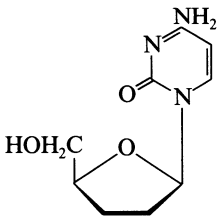
$C_{41}H_{58}O_2$ M 582.908
Constit. of *Erythrobacter longus*.

19′-Aldehyde, 9′-E-isomer: [119188-87-3]. ***(9′E)-3′,4′-Didehydro-1′,2′-dihydro-3R-hydroxy-1′-methoxy-β,ψ-caroten-19′-al***
$C_{41}H_{56}O_3$ M 596.892
Constit. of *E. longus*.

Takaichi, S. *et al*, *Phytochemistry*, 1988, **27**, 3605.

2′,3′-Dideoxycytidine, 9CI D-80152

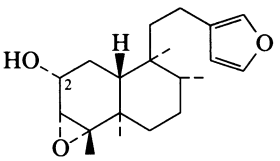
DDC



$C_9H_{13}N_3O_3$ M 211.220
Antiviral agent. Potentially of use against HIV infection. Mp 231-232° (214-217°). $[\alpha]_D^{20}$ +90° (c, 0.5 in H_2O), $[\alpha]_D$ +105.9° (c, 0.53 in MeOH).

Horwitz, J.P. *et al*, *J. Org. Chem.*, 1967, **32**, 817 (*synth*)
Mitsuya, H. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, (*London*), 1986, **83**, 1911 (*pharmacol*)
Mitsuya, H. *et al*, *Nature* (*London*), 1987, **325**, 773.
Okabe, M. *et al*, *J. Org. Chem.*, 1988, **53**, 4780 (*synth, ir, pmr, ms*)

ent-3β,4β;15,16-Diepoxy-13(16),14-clerodadien-2β-ol D-80153



$C_{20}H_{30}O_3$ M 318.455
Constit. of *Baccharis boliviensis*. Gum. $[\alpha]_D^{24}$ +8° (c, 5.65 in $CHCl_3$).

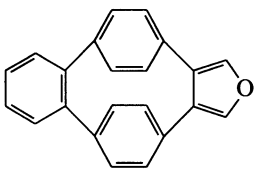
2-Me ether: ent-3β,4β;15,16-*Diepoxy*-2β-*methoxy*-13(16),14-*clerodadiene*
$C_{21}H_{32}O_3$ M 332.482
Constit. of *B. boliviensis*. Gum.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

4,7:12,15-Diethenobenzo[7,8]cyclo-dodeca[1,2-*c*]furan, 9CI D-80154

Benzofurano[c][*2.2*]*paracyclophane*

[111615-65-7]

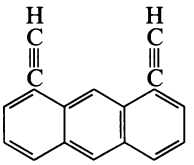


$C_{22}H_{14}O$ M 294.352
Cryst. (heptane). Mp 275° dec.

Chan, C.W. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 462 (*synth, uv, pmr*)

1,8-Diethynylanthracene D-80155

[78053-58-4]

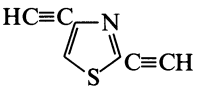


$C_{18}H_{10}$ M 226.277
Yellow plates (toluene). Mp 150° dec.

Katz, H.E., *J. Org. Chem.*, 1989, **54**, 2179 (*synth, pms, cmr*)

2,4-Diethynylthiazole D-80156

[113705-26-3]



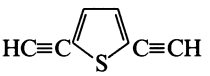
C_7H_3NS M 133.173
Oil. Unstable, darkened on standing.

▷ Potentially explosive.

Neenan, T.X. *et al*, *J. Org. Chem.*, 1988, **53**, 2489 (*synth, pmr, ms, haz*)

2,5-Diethynylthiophene D-80157

[79109-72-1]



C_8H_4S M 132.186
Liq. $Bp_{0.1}$ 40°.

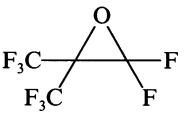
▷ Potentially explosive.

Okuhara, K., *Bull. Chem. Soc. Jpn.*, 1981, **54**, 2045 (*synth, ms, ir*)
Neenan, T.X. *et al*, *J. Org. Chem.*, 1988, **53**, 2489 (*synth, ir, pmr, cmr, haz*)

2,2-Difluoro-3,3-bis(trifluoromethyl) oxirane, 9CI D-80158

1,2-Epoxy-1,1,3,3,3-pentafluoro-2-(trifluoromethyl)propane, 8CI. 1,2-Epoxyperfluoroisobutene

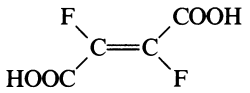
[707-13-1]



C_4F_8O M 216.031
Mp −122°. Bp 3°, Bp 6-7°.

Knunyants, I.L. *et al*, *Khim. Geterotsikl. Soedin.*, 1966, 873 (*synth, F-19 nmr*)
Croft, T.S., *J. Fluorine Chem.*, 1976, **7**, 438 (*synth, F-19 nmr*)

1,2-Difluoro-2-butenedioic acid D-80159



(*E*)-*form*

$C_4H_2F_2O_4$ M 152.054

(***E***)-***form*** [2714-32-1]
Difluorofumaric acid
Cryst. (H_2O). Mp 268-270°.

(***Z***)-***form*** [685-64-3]
Difluoromaleic acid
Cryst. (Me_2CO/C_6H_6). Mp 219-220°.

Anilinium salt: Mp 177-178.5°.

S-Benzylthiouronium salt: [15514-25-7].
Mp 231-232°.

Di-Me ester: [39774-02-2].
$C_6H_6F_2O_4$ M 180.108
Bp 153°.

Di-Et ester: [815-97-4].
$C_8H_{10}F_2O_4$ M 208.161
Bp_3 67°.

Anhydride: [669-78-3]. *3,4-Difluoro-2,5-furandione, 9CI.*
Difluoromaleic anhydride
$C_4F_2O_3$ M 134.039
Mp 20°. Bp 128°. n_D^{25} 1.4197.

Raasch, M.S. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 2678 (*anhydride*)
Kobrina, L.S. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1972, **8**, 2209 (*synth, deriv, uv, F nmr*)

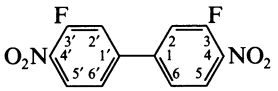
3,3-Difluoro-1,2-diiodocyclopropene, 9CI D-80160

1,2-Diiodo-3,3-difluorocyclopropene
[56830-73-0]

$C_3F_2I_2$ M 327.839
Bp_{35} 82-85°. n_D^{25} 1.5920.

Sepiol, J. *et al*, *J. Org. Chem.*, 1975, **40**, 3791 (*synth, F-19 nmr, ir*)

3,3′-Difluoro-4,4′-dinitrobiphenyl D-80161



$C_{12}H_6F_2N_2O_4$ M 280.187
Cryst. (MeOH). Mp 197.5-198.5°.

Fletcher, T.L. *et al*, *J. Org. Chem.*, 1960, **25**, 1342.

4,4′-Difluoro-2,2′-dinitrobiphenyl D-80162

[316-00-7]
$C_{12}H_6F_2N_2O_4$ M 280.187
Cryst. (C_6H_6). Mp 168-169°.

Shaw, F.R. *et al*, *J. Chem. Soc.*, 1932, 509 (*synth*)
Protiva, M. *et al*, *Collect. Czech. Chem. Commun.*, 1986, **51**, 698 (*uv, ir, pmr, ms*)

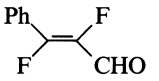
5,5′-Difluoro-2,2′-dinitrobiphenyl D-80163

[41860-49-5]
$C_{12}H_6F_2N_2O_4$ M 280.187
Cryst. (EtOH). Mp 121°.

Dickerson, D.R. *et al*, *J. Fluorine Chem.*, 1973, **3**, 113 (*synth*)

2,3-Difluoro-3-phenyl-2-propenal, 9CI D-80164

2,3-Difluorocinnamaldehyde



(*E*)-*form*

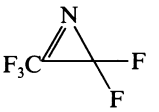
$C_9H_6F_2O$ M 168.143

(***E***)-***form*** [113894-39-6]
Yellow cryst. (hexane). Mp 32.0-33.0°.

Matsuo, N. *et al*, *J. Org. Chem.*, 1988, **53**, 2304 (*synth, pmr, F-19 nmr, ms*)

2,2-Difluoro-3-(trifluoromethyl)-2*H*-azirine, 9CI, 8CI D-80165

*Perfluoro(3-methyl-2*H*-azirine)*
[3291-42-7]

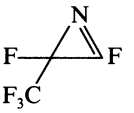


C_3F_5N M 145.032
Pale yellow oil. Bp −19.8°.

Cleaver, C.S. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 3716 (*synth, ir, F-19 nmr, ms*)
Banks, R.E. *et al*, *J. Chem. Soc. C*, 1966, 2304 (*synth, ir, F-19 nmr*)

2,3-Difluoro-2-(trifluoromethyl)-2*H*-azirine, 8CI D-80166

*Perfluoro(2-methyl-2*H*-azirine). Pentafluoro-2-azetine*
[3291-41-6]

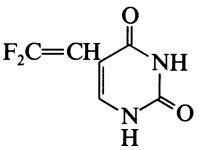


C_3F_5N M 145.032
Bp −15.5°, Bp −17°. Isomerises in glass or with moisture. Polymerises in contact with metal containers.

Cleaver, C.S. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 3716 (*synth, ir, F-19 nmr, ms*)
Banks, R.E. *et al*, *J. Chem. Soc. C*, 1966, 2304 (*synth, F-19 nmr*)

5-(2,2-Difluorovinyl)uracil D-80167

[108711-79-1]



$C_6H_4F_2N_2O_2$ M 174.107
Cryst. (MeOH/EtOH). Mp 288-292°.

1-(2-Deoxy-α-D-ribofuranosyl): [108742-87-6].
$C_{11}H_{12}F_2N_2O_5$ M 290.223
Mp 173-174°.

1-(2-Deoxy-β-D-ribofuranosyl): [108711-80-4]. *5-(2,2-Difluorovinyl)-2′-deoxyuridine*
$C_{11}H_{12}F_2N_2O_5$ M 290.223

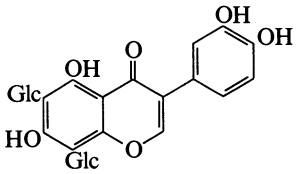
Active against Herpes simplex virus type 1 (HSV-1). Mp 152°.

Babek, M. *et al*, *J. Med. Chem.*, 1987, **30**, 1494 (*synth*, *pmr*)

6,8-Di-*C*-glucosyl-3′,4′,5,7-tetrahydroxy-isoflavone D-80168

6,8-Di-C-glucopyranosylorobol

[76436-69-6]

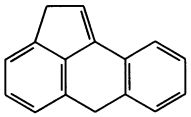


$C_{27}H_{30}O_{18}$ M 642.523

Isol. from bark of *Dalbergia nitidula*. Yellow amorph. solid. Mp 183-186°.

Van Heerden, F.R. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1980, 2463 (*isol*, *cmr*, *struct*)

2,6-Dihydroaceanthrylene D-80169



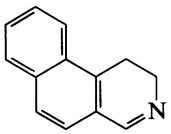
$C_{16}H_{12}$ M 204.271

Pale yellow cryst. (CH_2Cl_2/hexane). Mp 111°.

Rabideau, P.W. *et al*, *J. Org. Chem.*, 1988, **53**, 589 (*synth*, *pmr*)

1,2-Dihydrobenz[f]isoquinoline D-80170

[23950-51-8]



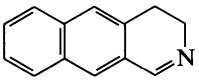
$C_{13}H_{11}N$ M 181.237

B,HCl: [112576-40-6].
Cryst. Mp 190-191°.

Young, S.D. *et al*, *J. Org. Chem.*, 1988, **53**, 1114 (*synth*, *pmr*, *cmr*, *ms*)

3,4-Dihydrobenz[*g*]isoquinoline D-80171

[112576-38-2]



$C_{13}H_{11}N$ M 181.237

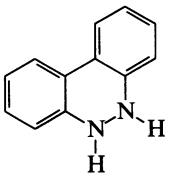
Cryst.

B,HCl: [112576-39-3].
Cryst. Mp 225-229°.

Young, S.D. *et al*, *J. Org. Chem.*, 1988, **53**, 1114 (*synth*, *pmr*, *ms*)

5,6-Dihydrobenzo[*c*]cinnoline, 9CI D-80172

[52125-81-2]



$C_{12}H_{10}N_2$ M 182.224

Cryst. Mp 122°.

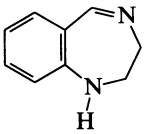
Mono-Ac:
$C_{14}H_{12}N_2O$ M 224.262
Needles (cyclohexane). Mp 114°.

Di-Ac:
$C_{16}H_{14}N_2O_2$ M 266.299
Leaflets (EtOH aq.). Mp 170°.

Wittig, G. *et al*, *Chem. Ber.*, 1955, **88**, 234 (*derivs*, *synth*)
Etienne, A. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 292 (*synth*, *derivs*)
Mugnier, Y. *et al*, *J. Org. Chem.*, 1988, **53**, 5781 (*synth*)

2,3-Dihydro-1*H*-1,4-benzodiazepine, 9CI D-80173

[5945-91-5]



$C_9H_{10}N_2$ M 146.191

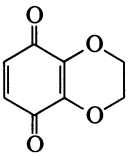
Cryst. (EtOH). Mp 253° (244-246°).

Uskokovic, M. *et al*, *J. Org. Chem.*, 1962, **27**, 3606 (*synth*, *ir*, *uv*)
Betakis, E. *et al*, *Synthesis*, 1988, 820 (*synth*, *ir*, *uv*, *pmr*)

2,3-Dihydro-1,4-benzodioxin-5,8-dione, 9CI D-80174

2,3-Ethylenedioxy-1,4-benzoquinone

[42965-39-9]



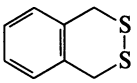
$C_8H_6O_4$ M 166.133

Red needles (EtOAc/hexane). Mp 158-159.5° (153-154°).

Bowman, C. *et al*, *J. Med. Chem.*, 1973, **16**, 988 (*synth*)
Hayakawa, K. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1988, 511 (*synth*, *pmr*, *ms*)

1,4- Dihydro-2,3-benzodithiin, 9CI D-80175

[3886-39-3]

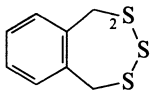


$C_8H_8S_2$ M 168.283

Needles (MeOH). Mp 77-78° (80°).

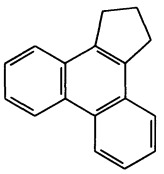
Lüttringhaus, A. *et al*, *Angew. Chem.*, 1955, **67**, 304 (*synth*)
Milligan, B. *et al*, *J. Chem. Soc.*, 1965, 2901 (*synth*, *pmr*)

1,5-Dihydro-2,3,4-benzotrithiepin, 9CI **D-80176**
2,3,4-Benzotrithiepin
[3354-86-7]



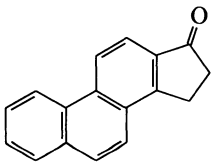
$C_8H_8S_3$ M 200.349
Plates (pet. ether). Mp 101-102°.
2-Oxide:
$C_8H_8OS_3$ M 216.349
Yellow prisms (EtOAc). Mp 133°.
Milligan, B. *et al*, *J. Chem. Soc.*, 1965, 2901 (*synth, ir, pmr*)

2,3-Dihydro-1*H*-cyclopenta[*l*] phenanthrene, 9CI **D-80177**
9,10-Cyclopentenophenanthrene
[723-98-8]



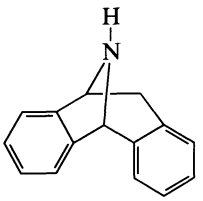
$C_{17}H_{14}$ M 218.298
Cryst. (EtOH). Mp 152.5-153.5°.
Cope, A.C. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 2547 (*synth*)
Wood, C.S. *et al*, *J. Org. Chem.*, 1964, **29**, 3373 (*synth*)
Penn, J.H. *et al*, *J. Org. Chem.*, 1989, **54**, 601 (*synth*)

15,16-Dihydro-17*H*-cyclopenta[*a*] phenanthren-17-one, 8CI **D-80178**
[786-66-3]



$C_{17}H_{20}O$ M 240.344
Solid (EtOAc). Mp 201-202°.
Coombs, M.M., *J. Chem. Soc. C*, 1966, 955 (*synth*)
Lee, H. *et al*, *J. Org. Chem.*, 1988, **53**, 4253 (*synth, pmr*)

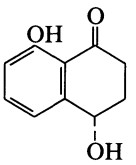
10,11-Dihydro-5*H*-dibenzo[*a,d*] cyclohepten-5,10-imine, 9CI **D-80179**



$C_{15}H_{13}N$ M 207.274
(±)-*form* [50537-17-2]
Cryst. (CH_2Cl_2/pet. ether). Mp 111.5-114° (120°).
Lamanec, T.R. *et al*, *J. Org. Chem.*, 1988, **53**, 1768 (*synth*)

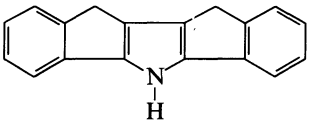
1,4-Dihydrodibenzothiophene **D-80180**
[109644-16-8]
$C_{12}H_{10}S$ M 186.277
Cryst. Mp 76°. Bp_6 160-165°.
Gilman, H. *et al*, *J. Org. Chem.*, 1938, **3**, 108 (*synth*)
Francisco, M.A. *et al*, *J. Org. Chem.*, 1988, **53**, 596 (*synth, pmr, ms*)

3,4-Dihydro-4,8-dihydroxy-1(2*H*)-naphthalenone **D-80181**
Regiolone
[54712-38-8]



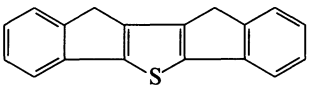
$C_{10}H_{10}O_3$ M 178.187
Constit. of *Juglans regia*. Cryst. (pet. ether). Mp 73°. $[\alpha]_D$ −3.3° (c, 0.077 in EtOH).
Talapatra, S.K. *et al*, *Phytochemistry*, 1988, **27**, 3929.

10,11-Dihydro-5*H*-diindeno[1,2-*b*;2′,1′-*d*] pyrrole, 9CI **D-80182**
[7099-31-2]



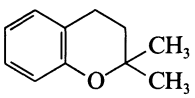
$C_{18}H_{13}N$ M 243.307
Cryst. (toluene under Ar). Mp 275° dec.
N-*Ph:* [115679-37-3].
$C_{24}H_{17}N$ M 319.405
Mp 169°.
Baierweck, P. *et al*, *Chem. Ber.*, 1988, **121**, 2195 (*synth, pmr, cmr*)

10,11-Dihydrodiindeno[1,2-*b*:2′,1′-*d*] thiophene, 9CI **D-80183**
[7099-33-4]



$C_{18}H_{12}S$ M 260.359
Cryst. ($CHCl_3$). Mp 288°.
Baierweck, P. *et al*, *Chem. Ber.*, 1988, **121**, 2195 (*synth, cmr*)
Czogalla, C.D. *et al*, *Phosphorus Sulfur*, 1988, **35**, 127 (*synth*)

3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran, 9CI **D-80184**
2,2-Dimethylchroman, 8CI
[1198-96-5]



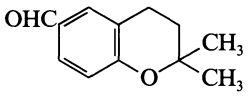
$C_{11}H_{14}O$ M 162.231
Yellow oil with spicy odour. d_4^{20} 1.02. $Bp_{11.5}$ 98-98.5°.
Claisen, L., *Ber.*, 1921, **54**, 200 (*synth*)
Shriner, R.L. *et al*, *J. Org. Chem.*, 1939, **4**, 575 (*synth*)

Frater, G. *et al*, *Helv. Chim. Acta*, 1967, **50**, 255 (*synth*)
Miller, J.A. *et al*, *J. Chem. Soc. C*, 1968, 1837 (*synth*)
Bolzoni, L. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1978, **17**, 684 (*synth*)
Camps, F. *et al*, *Synthesis*, 1979, 126 (*synth*)
Fatope, M.O. *et al*, *J. Med. Chem.*, 1987, **30**, 1973 (*synth, ir, pmr*)

3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-carboxaldehyde, 9CI D-80185

2,2-Dimethyl-6-chromancarboxaldehyde. 6-Formyl-2,2-dimethylchroman

[61370-75-0]



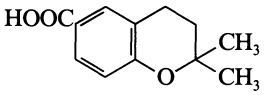
$C_{12}H_{14}O_2$ M 190.241
Liq. Bp_2 110-114°.

Knight, D.W. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1979, 30 (*synth, ir, pmr*)
Fatope, M.O. *et al*, *J. Med. Chem.*, 1987, **30**, 1973 (*synth, pmr*)

3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-carboxylic acid, 9CI D-80186

2,2-Dimethyl-6-chromancarboxylic acid

[2039-47-6]



$C_{12}H_{14}O_3$ M 206.241
Cryst. (MeOH aq.). Mp 184° (177-178°).

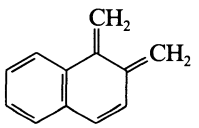
p-*Bromophenacyl ester:* Mp 147-148°.

Lauer, W.M. *et al*, *J. Am. Chem. Soc.*, 1943, **65**, 289 (*synth*)
Fatope, M.O. *et al*, *J. Med. Chem.*, 1987, **30**, 1973 (*synth, ir, pmr, ms*)

1,2-Dihydro-1,2-dimethylenenaphthalene D-80187

1,2-Dihydro-1,2-bis(methylene)naphthalene, 9CI. 1,2-Naphthalenequinodimethide

[41182-10-9]



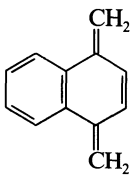
$C_{12}H_{10}$ M 154.211
Transient species detected by flow pmr.

Cava, M.P. *et al*, *J. Org. Chem.*, 1962, **27**, 755.
Trahanovsky, W.S. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6579.

1,2-Dihydro-1,4-dimethylenenaphthalene D-80188

1,4-Dihydro-1,4-bis(methylene)naphthalene, 9CI. 1,4-Naphthalenequinodimethide

[7545-39-3]



$C_{12}H_{10}$ M 154.211
Unstable intermediate trapped by Diels-Alder reaction or obs. by low temp. spectroscopy.

Cram, D.J. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 1088 (*synth*)
Williams, D.J. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 1436 (*synth, pmr, bibl*)
Pearson, J.M. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5034 (*synth, uv, ir*)

2,3-Dihydro-2,3-dimethylenenaphthalene, 8CI D-80189

2,3-Dihydro-2,3-bis(methylene)naphthalene, 9CI

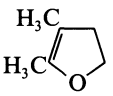
[39638-07-8]

$C_{12}H_{10}$ M 154.211
Reactive intermediate isolable at low temperature. Diene for cycloaddition reactions.

Cava, M. .P. *et al*, *J. Org. Chem.*, 1962, **27**, 755.
Gisin, M. *et al*, *Helv. Chim. Acta*, 1976, **59**, 2273 (*synth, uv*)
Bell, T.W. *et al*, *Tetrahedron Lett.*, 1980, **21**, 3299 (*dimers*)
Chew, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1984,, 911 (*synth, use*)

2,3-Dihydro-4,5-dimethylfuran D-80190

[1487-16-7]



$C_6H_{10}O$ M 98.144
Liq. Bp 106°.

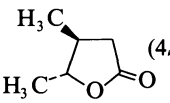
McGreer, D.E. *et al*, *Can. J. Chem.*, 1965, **43**, 1398 (*synth*)
Adam, W. *et al*, *J. Org. Chem.*, 1988, **53**, 1492 (*synth*)

Dihydro-4,5-dimethyl-2(3*H*)-furanone, 9CI D-80191

Updated Entry replacing D-03708

β-Methyl-γ-valerolactone. β,γ-Dimethylbutyrolactone. Tetrahydro-4,5-dimethyl-2-furanone

[6971-63-7]



(4*S*,5*R*)-*form*

$C_6H_{10}O_2$ M 114.144
Tobacco constit.

(4S,5R)-form [90026-46-3]
(+)-trans-*form*
$[\alpha]_D^{20}$ +56.9° (c, 1.8 in $CHCl_3$).

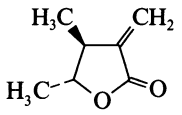
(4RS,5RS)-form [10150-95-5]
(±)-cis-*form*
Bp_{12} 95-97°.

(4RS,5SR)-form [10150-96-6]
(±)-trans-*form*
Bp_{12} 101-103°.

[110171-22-7]

Tokuda, M. *et al*, *J. Org. Chem.*, 1972, **37**, 1859 (*synth*)
Kimland, B. *et al*, *Phytochemistry*, 1973, **12**, 835 (*isol*)
Sucrow, W. *et al*, *Chem. Ber.*, 1975, **108**, 48 (*synth*)
Pyysalo, H. *et al*, *Finn. Chem. Lett.*, 1975, 129 (*cmr*)
Tsuzuki, K. *et al*, *Tetrahedron Lett.*, 1976, 4745 (*synth*)
Mattes, H. *et al*, *J. Med. Chem.*, 1987, **30**, 1948 (*synth, ir, pmr*)

Dihydro-4,5-dimethyl-3-methylene-2(3*H*)-furanone **D-80192**



$C_7H_{10}O_2$ M 126.155

(4S,5R)-form [110171-20-5]

(+)-trans-*form*

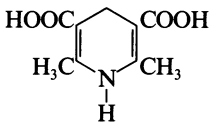
$[\alpha]_D^{20}$ +16.4° (c, 1.10 in $CHCl_3$).

[110171-21-6]

Mattes, H. *et al*, *J. Med. Chem.*, 1987, **30**, 1948 (*synth, ir, pmr*)

1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid, 9CI **D-80193**

[51595-68-7]



$C_9H_{11}NO_4$ M 197.190

Derivs. are vasodilators, hypotensives and oxidation inhibitors, heat stabilisers, etc.

Di-Me ester: [17438-14-1].

$C_{11}H_{15}NO_4$ M 225.244

Yellow needles (MeOH). Mp 225-227° (219-220°).

Di-Et ester: [1149-23-1].

$C_{13}H_{19}NO_4$ M 253.297

Yellow needles with green fluorescence (EtOH). Mp 183-185° (176-183°).

*Di-*tert*-butyl ester:* [55536-71-5].

$C_{17}H_{27}NO_4$ M 309.405

Cryst. (EtOH). Mp 142-144°.

Dibenzyl ester: [36138-79-1].

$C_{23}H_{23}NO_4$ M 377.439

Cryst. (EtOH). Mp 119-121°.

Dinitrile: [3274-36-0].

$C_9H_9N_3$ M 159.190

Yellowish plates (MeOH). Mp 232-233° (222°).

1-Me, di-Et ester: [14258-07-2].

$C_{14}H_{21}NO_4$ M 267.324

Cryst. (pet. ether). Mp 84-85°.

1-Me, dinitrile: [14258-16-3].

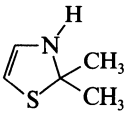
$C_{10}H_{11}N_3$ M 173.217

Cryst. (C_6H_6/pet. ether). Mp 132.5-133°.

Meyer, E., *J. Prakt. Chem.*, [2], 1908, **78**, 497 (*nitrile*)
Org. Synth., Coll. Vol., 2, 1943, 214 (*Et ester, synth*)
Kuthan, J. *et al*, *Collect. Czech. Chem. Commun.*, 1964, **29**, 1654 (*dinitrile*)
Brignell, P.J. *et al*, *J. Chem. Soc. B*, 1966, 1083 (*derivs, uv*)
Roomi, M.W., *J. Med. Chem.*, 1975, **18**, 457 (*esters, pharmacol*)
Lenstra, A.T.H. *et al*, *Bull. Soc. Chim. Belg.*, 1979, **88**, 133 (*Et ester, cryst struct*)
Kurfürst, A. *et al*, *Collect. Czech. Chem. Commun.*, 1983, **48**, 1422; 1984, **49**, 2893 (*derivs, uv, pmr*)

2,3-Dihydro-2,2-dimethylthiazole **D-80194**

2,2-Dimethylthiazolidine



C_5H_9NS M 115.199

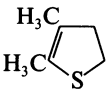
Potent inhibitor of platelet aggregation.

B,HCl: Mp 174-176°.

Mimura, T. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 1110 (*synth, pmr, pharmacol*)

2,3-Dihydro-4,5-dimethylthiophene **D-80195**

[113379-98-9]



$C_6H_{10}S$ M 114.211

Liq. Bp_{12} 42°. Stored at 0° under N_2.

1-Oxide: [113380-05-5].

$C_6H_{10}OS$ M 130.210

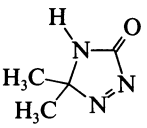
Liq.

Adam, W. *et al*, *J. Org. Chem.*, 1988, **53**, 1492 (*synth, pmr, ir, uv*)

4,5-Dihydro-5,5-dimethyl-3*H*-1,2,4-triazol-3-one, 9CI **D-80196**

5,5-Dimethyl-Δ^1*-1,2,4-triazolin-3-one*

[112700-85-3]



$C_4H_7N_3O$ M 113.119

Cryst. (Et_2O). Mp 84-87°.

N-*Benzoyl:*

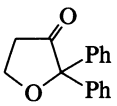
$C_{11}H_{11}N_3O_2$ M 217.227

Cryst. (EtOH). Mp 107-107.5°.

Schantl, J.G. *et al*, *Heterocycles*, 1987, **26**, 1439 (*synth*)
Schantl, J.G. *et al*, *J. Heterocycl. Chem.*, 1987, **24**, 1401 (*cryst struct, ir, uv, pmr, cmr, ms*)
Schantl, J.G. *et al*, *Synthesis*, 1987, 986 (*synth*)

Dihydro-2,2-diphenyl-2(3*H*)-furanone, 9CI **D-80197**

[101110-06-9]

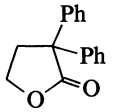


$C_{16}H_{14}O_2$ M 238.285

Needles (EtOH). Mp 74.5-75.5°.

Flavin, M.T. *et al*, *J. Med. Chem.*, 1987, **30**, 278 (*synth, pmr, ir, ms*)

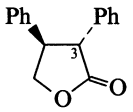
Dihydro-3,3-diphenyl-2(3*H*)-furanone, 9CI **D-80198**
α,α-Diphenyl-γ-butyrolactone
[956-89-8]



$C_{16}H_{14}O_2$ M 238.285
Prisms (MeOH/Me_2CO). Mp 80-81° (77-79°).

Morand, P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, **8**, 458 (*synth*)
Bocelli, G. *et al*, *J. Mol. Struct.*, 1982, **81**, 113 (*cryst struct*)
Kayser, M.M. *et al*, *Can. J. Chem.*, 1983, **61**, 439 (*synth, uv, pmr*)
Shibata, I. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 4000 (*synth, ir, ms, pmr*)

Dihydro-3,4-diphenyl-2(3*H*)-furanone, 9CI **D-80199**
α,β-Diphenyl-γ-butyrolactone
[25109-89-1]

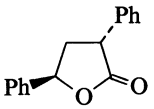


(3*R*,4*R*)-*form*

$C_{16}H_{14}O_2$ M 238.285
(3R,4R)-form [24435-71-0]
(−)-trans-*form*
Cryst. (EtOH). Mp 96.5-98°. $[\alpha]_D^{23}$ −196.7° (c, 0.231 in $CHCl_3$).
(3RS,4RS)-form
(±)-trans-*form*
Cryst. Mp 96-96.5°.

Berova, N. *et al*, *Tetrahedron*, 1969, **25**, 2301 (*synth, ir, uv, abs config*)
Fukuoka, S. *et al*, *J. Org. Chem.*, 1970, **35**, 3184 (*synth, ir*)

Dihydro-3,5-diphenyl-2(3*H*)-furanone, 9CI **D-80200**
α,γ-Diphenyl-γ-butyrolactone
[21034-29-7]



(3*RS*,5*RS*)-*form*

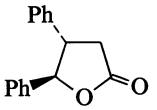
$C_{16}H_{14}O_2$ M 238.285
(3RS,5RS)-form [20272-26-8]
(±)-trans-*form*
Cryst. (Et_2O/hexane). Mp 74° (68-69°).
(3RS,5SR)-form [20272-24-6]
(±)-cis-*form*
Cryst. (Me_2CO/hexane). Mp 107-107.5°.
[94848-88-1]

Givens, R.S. *et al*, *J. Org. Chem.*, 1972, **37**, 4325 (*synth*)
Fujita, T. *et al*, *Aust. J. Chem.*, 1974, **27**, 2205 (*synth*)
Hussain, T.S.A.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 1480 (*synth, pmr*)

Dihydro-4,4-diphenyl-2(3*H*)-furanone, 9CI **D-80201**
β,β-Diphenyl-γ-butyrolactone
[67390-35-6]
$C_{16}H_{14}O_2$ M 238.285
Mp 109-110°.

Legagneur, F.S., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1948, **227**, 437 (*synth*)
Morand, P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 458 (*synth*)
Kayser, M.M. *et al*, *Can. J. Chem.*, 1983, **61**, 439 (*synth, uv, pmr*)

Dihydro-4,5-diphenyl-2(3*H*)-furanone, 9CI **D-80202**
2,3-Diphenyl-4-butanolide
[20453-83-2]



(3*RS*,4*RS*)-*form*

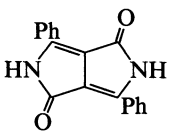
$C_{16}H_{14}O_2$ M 238.285
(3RS,4RS)-form [53861-52-2]
(±)-trans-*form*
No phys. props. reported.
(3RS,4SR)-form [5635-41-6]
(±)-cis-*form*
Needles(EtOAc). Mp 127-128°.
[69573-46-2]

Burns, W.D.P. *et al*, *J. Chem. Soc. C*, 1967, 1554 (*synth, uv, pmr*)
Heiba, E.I. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5905; 1974, **96**, 7977 (*synth*)
Schine, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 224 (*synth, pmr*)

Dihydro-5,5-diphenyl-2(3*H*)-furanone, 9CI **D-80203**
4,4-Diphenylbutyrolactone. 4,4-Diphenyl-4-butanolide
[7746-94-3]
$C_{16}H_{14}O_2$ M 238.285
Microcryst. (EtOH). Mp 91-92°.

Staab, H.A. *et al*, *Justus Liebigs Ann. Chem.*, 1966, **694**, 78 (*synth*)
King, G.S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1974, 1499 (*synth*)
Loozen, H.J.J. *et al*, *J. Org. Chem.*, 1975, **40**, 892 (*synth*)
Sturtz, G. *et al*, *Tetrahedron Lett.*, 1976, 47 (*synth*)
Miller, R.D. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 1508 (*synth*)
Fujimoto, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 3161 (*synth*)
Fukuzawa, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 475, 624 (*synth*)
Lehmann, J. *et al*, *Synthesis*, 1987, 1064 (*synth, ir, pmr*)

2,5-Dihydro-3,6-diphenylpyrrolo[3,4-*c*] pyrrole-1,4-dione, 9CI **D-80204**
Updated Entry replacing D-70204
*3,6-Diphenyl-2,5-diaza-1,4(2*H*,5*H*)-pentalenedione*



Pigment. Red powder, red cryst. (toluene or DMF). Mp >350°.

2,5-Di-Me: [96159-17-0].
$C_{20}H_{16}N_2O_2$ M 316.359
Orange cryst. ($PhNO_2$). Mp 236-238°.

2,5-Di-Et: [96159-13-6].
$C_{22}H_{20}N_2O_2$ M 344.412
Orange yellow needles (butanol). Mp 229-230°.

2-Butyl: [96159-00-1].
$C_{22}H_{20}N_2O_2$ M 344.412
Yellow cryst. (MeOH). Mp 250-252°.

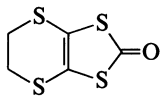
2,5-Dibenzyl: [96159-02-3].

$C_{32}H_{24}N_2O_2$ M 468.554
Orange yellow cryst. (DMF). Mp 290-292°.

Farnum, D.G. *et al*, *Tetrahedron Lett.*, 1974, 2549 (*synth*)
Eur. Pat., 133 156, (1984); *CA*, **102**, 186667 (*derivs*)
Closs, F. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 552 (*synth, uv*)
Potrawa, T. *et al*, *Chem. Ber.*, 1987, **120**, 1075 (*synth, derivs, uv, pmr*)

5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-one, 9CI D-80205

2,5,7,9-Tetrathiabicyclo[4.3.0]non-1(6)-en-8-one
[74962-29-1]

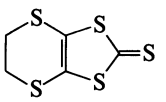


$C_5H_4OS_4$ M 208.350
Cryst. Mp 127-128°.

Hartke, K. *et al*, *Chem. Ber.*, 1980, **113**, 1898 (*synth, pmr, cmr, ir, uv*)
Varma, S.K. *et al*, *Synthesis*, 1987, 837 (*synth, pmr, cmr, ir, uv, ms*)

5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-thione, 9CI D-80206

2,5,7,9-Tetrathiabicyclo[4.3.0]non-1(6)-ene-8-thione
[59089-89-3]

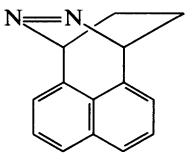


$C_5H_4S_5$ M 224.417
Cryst. ($CHCl_3$/EtOH). Mp 119-120°.

Maruno, M. *et al*, *J. Org. Chem.*, 1976, **41**, 1484 (*synth*)
Hartke, K. *et al*, *Chem. Ber.*, 1980, **113**, 1898 (*synth, pmr, cmr, ir*)
Varma, S.K. *et al*, *Synthesis*, 1987, 837 (*synth, pmr, cmr, ir, uv, ms*)

1,4-Dihydro-1,4-ethanonaphtho[1,8-*de*][1,2]diazepine, 9CI D-80207

[52720-26-0]

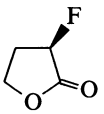


$C_{14}H_{12}N_2$ M 208.262
Pale yellow cryst. ($CHCl_3$/hexane) or glassy solid. Mp 123-125°.

Watson, C.R. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 2551 (*synth, uv, pmr*)
Burnett, M.N. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2527 (*synth, uv, use*)

Dihydro-3-fluoro-2(3*H*)-furanone D-80208

2-Fluoro-γ-butyrolactone



(*R*)-*form*

$C_4H_5FO_2$ M 104.081

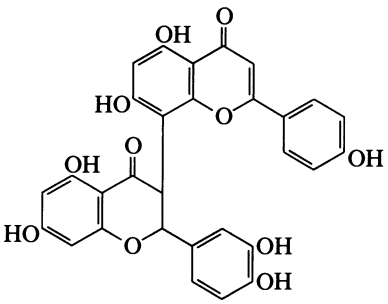
(*R*)-*form* [86677-74-9]
Volatile oil. $[\alpha]_D^{22}$ +50.3° (c, 0.95 in $CHCl_3$).

[86677-82-9]

Shiuey, S.-J. *et al*, *J. Org. Chem.*, 1988, **53**, 1040 (*synth, ir, pms, ms*)

2,3-Dihydro-3′,4′,4″,5,5″,7,7″-heptahydroxy-3,8′-biflavone D-80209

3′,4′,4″,5,5″,7,7″-Heptahydroxy[3,8]flavanonylflavone
[119459-71-1]

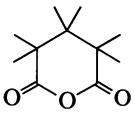


$C_{30}H_{20}O_{11}$ M 556.481
Constit. of *Garcinea nervosa*. Yellow cryst. (MeOH). Mp 232-234°.

Babu, V. *et al*, *Phytochemistry*, 1988, **27**, 3332.

Dihydro-3,3,4,4,5,5-hexamethyl-2*H*-pyran-2,6(3*H*)-dione, 9CI D-80210

3,3,4,4,5,5-Hexamethyltetrahydropyran-2,6-dione

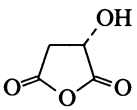


$C_{11}H_{18}O_3$ M 198.261
Cryst. by subl. Mp 174-175°.

Baran, J. *et al*, *J. Org. Chem.*, 1988, **53**, 4626 (*synth, ir, pmr, cmr, ms*)

Dihydro-3-hydroxy-2,5-furandione, 9CI D-80211

Hydroxysuccinic anhydride. Malic anhydride
[1121-34-2]



(*S*)-*form*

$C_4H_4O_4$ M 116.073
Freq. confused in CA with maleic anhydride.

(*S*)-*form*

Me ether: [117237-88-4]. *Dihydro-3-methoxy-2,5-furandione, 9CI. 2-Methoxysuccinic anhydride*
$C_5H_6O_4$ M 130.100
Bp_{15} 125°. $[\alpha]_D^{20}$ −104° (c, 2 in C_6H_6).

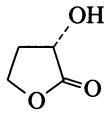
tert-Butyl ether: [117237-89-5]. *3-(1,1-Dimethylethoxy)dihydro-2,5-furandione, 9CI.* 2-tert-*Butoxysuccinic anhydride*
$C_8H_{12}O_4$ M 172.180
Cryst. (toluene/hexane). Mp 64°. $[\alpha]_D^{20}$ −51.5°.

(±)-*form*
Cryst. (Et_2O). Sol. H_2O. Mp 75-76°.

Purdie, T. *et al*, *J. Chem. Soc.*, 1910, **97**, 1524 (*derivs*)
Denhorn, W.S., *J. Chem. Soc.*, 1913, **103**, 1861 (*synth*)
Polonski, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 629 (*derivs*)

Dihydro-3-hydroxy-2(3*H*)-furanone D-80212

2-Hydroxy-γ-butyrolactone



(*S*)-*form*

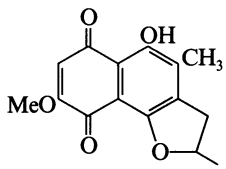
$C_4H_6O_3$ M 102.090

(***S***)-***form*** [52079-23-9]
Liq. $Bp_{0.1}$ 95°. $[\alpha]_D^{25}$ −65.2°.

Abdallah, M.A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 888 (*synth*)
Shiuey, S.-J. *et al*, *J. Org. Chem.*, 1988, **53**, 1040 (*synth, ir, pmr, ms*)

2,3-Dihydro-5-hydroxy-8-methoxy-2,4-dimethylnaphtho[1,2-b]furan-6,9-dione D-80213

[115401-70-2]

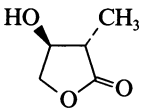


$C_{15}H_{14}O_5$ M 274.273
Metab. of *Fusarium solani*. Red cryst. (EtOAc). Mp 220-224°.

Tatum, J.H. *et al*, *Phytochemistry*, 1989, **28**, 283.

Dihydro-4-hydroxy-3-methyl-2(3*H*)-furanone D-80214

2-Methyl-3,4-dihydroxybutanoic acid 1,4-lactone



$C_5H_8O_3$ M 116.116

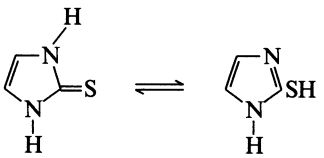
(***3S,4S***)-***form*** [112138-02-0]
(−)-trans-form
Liq. Bp_{15} 163-165°. $[\alpha]_D^{20}$ −58° (c, 2.87 in MeOH).

Larcheveque, M. *et al*, *Tetrahedron*, 1987, **43**, 2303 (*synth, pmr, cmr, ms*)

1,3-Dihydro-2*H*-imidazole-2-thione, 9CI D-80215

Imidazole-2-thione. 2-Mercaptoimidazole. Imidazole-2-thiol, 8CI

[872-35-5]



$C_3H_4N_2S$ M 100.144
Cryst. (H_2O). Mp 226-228°.

1-Me: see 1,3-*Dihydro*-1-*methyl*-2H-*imidazole*-2-*thione*, *D*-80221

S-*Me:* [7666-04-8]. *2-(Methylthio)-1*H*-imidazole, 9CI*
$C_4H_6N_2S$ M 114.171
Mp 142°.

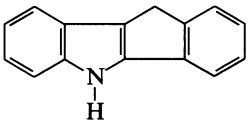
1,3-Di-Me: see 1,3-*Dihydro*-1-*methyl*-2H-*imidazole*-2-*thione*, *D*-80221

Marckwald, W., *Ber.*, 1892, **25**, 2354 (*synth*)
Akobori, S., *Ber.*, 1933, **66**, 151 (*synth*)
Simon, I.B. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1955, **25**, 1173 (*synth, deriv*)
Freeman, F. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2586 (*ir, pmr, cmr, uv, ms, cryst struct*)

5,10-Dihydroindeno[1,2-*b*]indole, 9CI D-80216

*Indeno[1,2-*b*]indole*

[3254-91-9]



$C_{15}H_{11}N$ M 205.259
Needles (MeOH). Mp 227-228°.

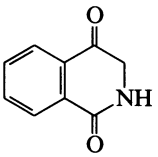
N-Me:
$C_{16}H_{13}N$ M 219.285
Cryst. (EtOH). Mp 153-154°.

Armit, J.W. *et al*, *J. Chem. Soc.*, 1922, 827.
Kahaoka, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1966, **14**, 934 (*synth*)

2,3-Dihydro-1,4-isoquinolinedione D-80217

Tetrahydroisoquinolinedione

[31053-30-2]



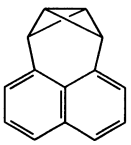
$C_9H_7NO_2$ M 161.160
Mp >300°.

Caswell, R.L. *et al*, *J. Org. Chem.*, 1961, **26**, 4175 (*synth*)
Caswell, R.L. *et al*, *J. Heterocycl. Chem.*, 1970, **7**, 1205 (*uv*)

2,3-Dihydro-1,2,3-metheno-1*H*-phenalene, 9CI D-80218

Naphtho[1,8]tricyclo[4.1.0.0^{2,7}]heptene. Naphthobicyclobutane

[40480-63-5]



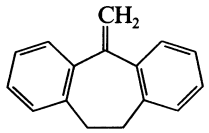
$C_{14}H_{10}$ M 178.233
Needles (pet. ether). Mp 76.5-77°.

Murata, I. *et al*, *Tetrahedron Lett.*, 1973, 47 (*synth, ms, uv, ir, pmr*)
Pagni, R.M. *et al*, *Tetrahedron Lett.*, 1973, 59 (*synth*)
Watson, C.R. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 2557 (*synth*)
Gleiter, R. *et al*, *Helv. Chim. Acta*, 1981, **64**, 1312 (*pe, struct*)

10,11-Dihydro-5-methylene-5*H*-dibenzo [*a,d*]cycloheptene, 9CI D-80219

3-Methylenedibenzsuberane

[2732-90-3]



$C_{16}H_{14}$ M 206.287

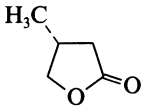
Cryst. (pet. ether). Mp 65-67°.

Triebs, W. *et al*, *Ber.*, 1950, **83**, 367 (*synth*)
Lamanec, T.R. *et al*, *J. Org. Chem.*, 1988, **53**, 1768 (*synth, pmr*)

Dihydro-4-methyl-2(3*H*)-furanone D-80220

3-Methyl-4-butanolide. 3-Methyl-γ-butyrolactone

[1679-49-8]



(*R*)-*form*

$C_5H_8O_2$ M 100.117

(*R*)-*form* [65284-00-6]
Bp_{45} 120°. $[\alpha]_D^{20}$ +24.0° (c, 3.32 in Et_2O).

(*S*)-*form* [64190-48-3]
Bp_{15} 87-89°. $[\alpha]_D$ −24.6° (neat).

(±)-*form* [70470-05-2]
d_4^{20} 1.058. Bp_{11} 76-76.5°. n_D^{20} 1.4339.

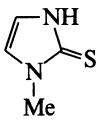
Seidel, C.F. *et al*, *Helv. Chim. Acta*, 1959, **42**, 1830 (*synth, ir*)
Leuenberger, H.G.W. *et al*, *Helv. Chim. Acta*, 1979, **62**, 455 (*synth, pmr*)
Mukaiyama, T. *et al*, *Chem. Lett.*, 1980, 635 (*synth*)
Mori, K. *et al*, *Tetrahedron*, 1983, **39**, 3107 (*synth, ir, pmr*)
Mattes, H. *et al*, *J. Med. Chem.*, 1987, **30**, 1948 (*synth, pmr, ir*)
Fuganti, C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3061 (*synth*)

1,3-Dihydro-1-methyl-2*H*-imidazole-2-thione, 9CI D-80221

Updated Entry replacing D-03892

1-Methylimidazole-2-thiol, 8CI. 2-Mercapto-1-methylimidazole. ***Methimazole,*** **BAN.** *Thiamazole, INN. Mercazolyl. Metimazol. Tapazole. Other proprietary names*

[60-56-0]



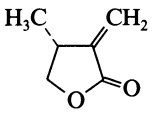
$C_4H_6N_2S$ M 114.171

Used in treatment of hyperthyroidism. Leaflets (EtOH). Mp 146-148°. Bp 280° dec.

▷ NI8615000.

Wohl, A. *et al*, *Ber.*, 1889, **22**, 1354 (*synth*)
Jones, R.G. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 4000 (*synth*)
Bowie, J.H. *et al*, *Aust. J. Chem.*, 1967, **20**, 1613 (*ms*)
Langer, P., *Endocrinology*, 1968, **83**, 1268 (*pharmacol*)
Aboul-Enein, H.Y. *et al*, *Anal. Profiles Drug Subst.*, 1979, **8**, 351 (*rev*)
Skellern, G.G. *et al*, *Xenobiotica*, 1981, **11**, 627 (*metab*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 835.
Raper, E.S. *et al*, *Acta Crystallogr., Sect. B*, 1983, **39**, 355 (*cryst struct*)
Anjaneyulu, B. *et al*, *J. Labelled Compd. Radiopharm.*, 1983, **20**, 951 (*synth*)
Merck Index, 10th Ed. Nos. 1983, 5844, 1983.
Cooper, D.S. *et al*, *Endocrinology*, 1984, **114**, 786 (*pharmacol*)
Balestrero, R.S. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 651 (*N*-15 *nmr, cmr*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 180 (*synonyms*)

Dihydro-4-methyl-3-methylene-2(3*H*)-furanone D-80222



(*R*)-*form*

$C_6H_8O_2$ M 112.128

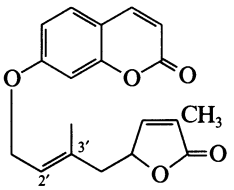
(*R*)-*form* [62322-50-3]
$[\alpha]_D^{20}$ +73.3° (6.17 in $CHCl_3$).

[110098-10-7]

Mattes, H. *et al*, *J. Med. Chem.*, 1987, **30**, 1948 (*synth, ir, pmr*)

7-[[4-(2,5-Dihydro-4-methyl-5-oxo-2-furanyl)-3-methyl-2-butenyl]oxy]-2*H*-1-benzopyran-2-one, 9CI D-80223

[53771-63-4]



$C_{19}H_{18}O_5$ M 326.348

Isol. from *Capnophyllum peregrinum*. Cryst. (MeOH). Mp 126°. $[\alpha]_D^{25}$ −26°.

2′,3′-Epoxide: [51559-34-3]. ***7-[[3-[(2,5-Dihydro-4-methyl-5-oxo-2-furanyl)methyl]-3-methyloxiranyl]methoxy]-2H-1-benzopyran-2-one,*** **9CI**
$C_{19}H_{18}O_6$ M 342.348
Mp 125°.

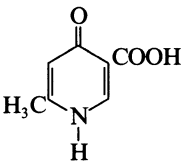
[51559-33-2]

Bohlmann, F. *et al*, *Chem. Ber.*, 1970, **103**, 3619; 1974, **107**, 1780 (*isol, uv, ir, pmr, struct*)

1,4-Dihydro-6-methyl-4-oxo-3-pyridinecarboxylic acid, 9CI D-80224

*6-Methyl-4(1*H*)-pyridone-3-carboxylic acid. 4-Hydroxy-6-methyl-3-pyridinecarboxylic acid*

[33821-58-8]



$C_7H_7NO_3$ M 153.137

Cryst. (H_2O). Mp 267°.

1-Me: [33821-59-9].
$C_8H_9NO_3$ M 167.164

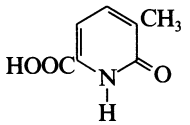
Cryst. (EtOH aq.). Mp 231-232°.

Kilbourn, E. *et al*, *J. Org. Chem.*, 1972, **37**, 1145 (*synth, deriv*)
Mittelbach, M. *et al*, *Synthesis*, 1988, 479 (*synth*)

1,6-Dihydro-3-methyl-6-oxo-2-pyridinecarboxylic acid, 9CI **D-80225**

3-Methyl-6-carboxy-2-pyridone

[115185-81-4]



$C_7H_7NO_3$ M 153.137
Cryst. (MeOH). Mp 209-210°.

Konno, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4807 (*synth, ir, uv, pmr*)

1,6-Dihydro-5-methyl-6-oxo-2-pyridinecarboxylic acid, 9CI **D-80226**

5-Methyl-6-carboxy-2-pyridone

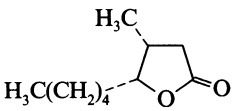
[115185-79-0]

$C_7H_7NO_3$ M 153.137
Cryst. Mp 295° dec.

Konno, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4807 (*synth, ir, uv, pmr*)

Dihydro-4-methyl-5-pentyl-2(3*H*)-furanone **D-80227**

Tetrahydro-4-methyl-5-pentyl-2-furanone. 3-Methyl-4-nonanolide. Cognac lactone



$C_{10}H_{18}O_2$ M 170.251

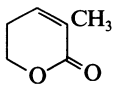
(3RS,4RS)-form

(±)-cis-*form*

Found in cognac, presumably in an enantiomeric form. Oil.

Jefford, C.W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1362 (*synth, ir, pmr, cmr, bibl*)

5,6-Dihydro-3-methyl-2*H*-pyran-2-one **D-80228**



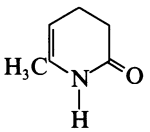
$C_6H_8O_2$ M 112.128
Liq. Bp_2 42-44° (bulb) .

Hofstraat, R.G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2315 (*synth, ms, ir, pmr*)

3,4-Dihydro-6-methyl-2(1*H*)-pyridinone, 9CI **D-80229**

1,2,3,4-Tetrahydro-6-methyl-2-oxopyridine

[10333-14-9]



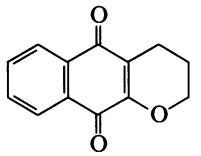
C_6H_9NO M 111.143

Cryst. (Et_2O). Mp 108°.

Schumann, D. *et al*, *Justus Liebigs Ann. Chem.*, 1983, 220 (*synth, ir, uv, pmr, cmr, ms*)
Knapp, S. *et al*, *J. Org. Chem.*, 1988, **53**, 4006 (*synth, ir*)

2*H*-3,4-Dihydronaphtho[2,3-*b*]pyran-5,10-dione **D-80230**

[106261-85-2]



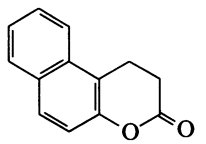
$C_{13}H_{10}O_3$ M 214.220
Yellow needles (MeOH). Mp 219-220°.

Hayashi, T. *et al*, *J. Med. Chem.*, 1987, **30**, 2005 (*synth, ir, uv, pmr*)

1,2-Dihydro-3*H*-naphtho[2,1-*b*]pyran-3-one, 9CI **D-80231**

3,4-Dihydro-5,6-benzocoumarin

[5690-03-9]



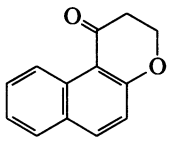
$C_{13}H_{10}O_2$ M 198.221
Solid (hexane). Mp 54-55°.

Das Gupta, A.K. *et al*, *J. Chem. Soc. C*, 1969, 2618 (*synth, ir, uw*)

2,3-Dihydro-1*H*-naphtho[2,1-*b*]pyran-1-one, 9CI **D-80232**

7,8-Benzochromanone

[4707-36-2]



$C_{13}H_{10}O_2$ M 198.221
Light yellow needles (EtOH) or rhombic tablets. Mp 108° (104.5°, 96-98°). $Bp_{0.5}$ 156-160°.

Oxime:
$C_{13}H_{11}NO_2$ M 213.235
Plates (EtOH). Mp 144-144.5° (134°).

Semicarbazone: Needles. Mp 276° (259-260°)dec.

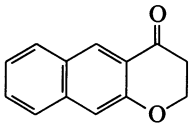
2,4-Dinitrophenylhydrazone: Red cryst. Mp 302°.

Pfeiffer, P. *et al*, *J. Chem. Soc.*, 1917, **112**, 661 (*synth*)
Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1958, 325 (*synth*)
Cagniant, P. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 3249 (*synth*)
Kasturi, T.R. *et al*, *Indian J. Chem.*, 1970, **8**, 203 (*synth, ir*)
Sharma, S.D. *et al*, *Indian J. Chem., Sect. B*, 1984, **23**, 518 (*synth, ir, pmr*)
Subramanian, L.M. *et al*, *Synthesis*, 1984, 1063 (*synth*)
Ravikumar, K. *et al*, *Acta Crystallogr., Sect. C*, 1986, **42**, 1423 (*cryst struct*)

2,3-Dihydro-4*H*-naphtho[1,2-*b*]pyran-4-one, 9CI **D-80233**

6,7-Benzochromanone

[16563-51-2]



$C_{13}H_{10}O_2$ M 198.221

Pale yellow needles (MeOH). Mp 131-132°.

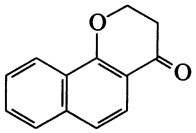
2,4-Dinitrophenylhydrazone: Red cryst. ($CHCl_3$/MeOH). Mp 252-254° dec.

Bell, K.H. *et al*, *Aust. J. Chem.*, 1963, **16**, 690 (*synth*)

2,3-Dihydro-4*H*-naphtho[2,3-*b*]pyran-4-one, 9CI **D-80234**

5,6-Benzochromanone

[4707-39-5]



$C_{13}H_{10}O_2$ M 198.221

Yellow needles (EtOH), cryst. (C_6H_6/pet. ether). Mp 50-51° (44°). $Bp_{2.5}$ 160-161°. $n_D^{23.2}$ 1.6556.

Oxime:

$C_{13}H_{11}NO_2$ M 213.235

Cryst. (EtOH). Mp 112°.

2,4-Dinitrophenylhydrazone: Brilliant scarlet solid. Mp 312°.

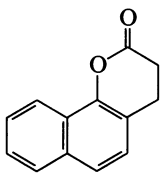
Semicarbazone: Light yellow plates (EtOH). Mp 227° dec.

Bachman, G.B. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 2341 (*synth*)
Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1958, 325 (*synth*)
Bell, K.H. *et al*, *Aust. J. Chem.*, 1963, **16**, 101 (*synth*)
Cagniant, P. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 3249 (*synth*)
Shenker, G.C. *et al*, *Synthesis*, 1983, 310 (*synth, ir, uv*)

3,4-Dihydro-2*H*-naphtho[1,2-*b*]pyran-2-one, 8CI **D-80235**

3,4-Dihydro-7,8-benzocoumarin

[5690-05-1]



$C_{13}H_{10}O_2$ M 198.221

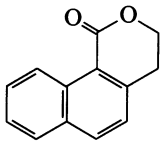
Mp 75-76°.

Das Gupta, A.K. *et al*, *J. Chem. Soc. C*, 1969, **18**, 2618 (*synth, uw, ir*)
Sarma, A.S., *Indian J. Chem.*, 1971, **9**, 93 (*synth, uw*)

3,4-Dihydro-1*H*-naphtho[1,2-*c*]pyran-3-one **D-80236**

3,4-Dihydro-7,8-benzoisocoumarin

[54959-66-9]



$C_{13}H_{10}O_2$ M 198.221

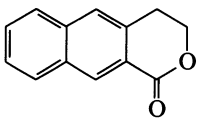
Solid. Mp 106°.

Bhide, B.H. *et al*, *Chem. Ind.* (*London*), 1974, 773 (*synth, uw, pmr*)

3,4-Dihydro-1*H*-naphtho[2,3-*c*]pyran-1-one, 9CI **D-80237**

3,4-Dihydro-6,7-benzoisocoumarin

[54959-67-0]



$C_{13}H_{10}O_2$ M 198.221

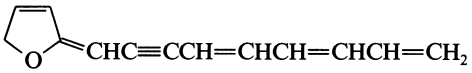
Solid. Mp 101°.

Bhide, B.H. *et al*, *Chem. Ind.* (*London*), 1974, 773 (*synth, uw, pmr*)

2,5-Dihydro-2-(4,6,8-nonatrien-2-ynylidene)furan, 9CI **D-80238**

2-(4,6,8-Nonatrien-2-ynylidene)-2,5-dihydrofuran

[13894-85-4]



$C_{13}H_{12}O$ M 184.237

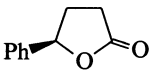
Isol. from roots of *Centaurea pullata* and *C. ferax*. Yellowish oil. λ_{max} 359, 379 nm (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3544 (*isol, uv, ir, pmr, ms, struct*)

Dihydro-5-phenyl-2(3*H*)-furanone, 9CI **D-80239**

4-Phenyl-4-butanolide. γ-Phenylbutyrolactone

[1008-76-0]



(*R*)-*form*

$C_{10}H_{10}O_2$ M 162.188

(R)-form [111138-03-5]

$[\alpha]_D$ +16.3° (c, 0.89 in EtOH).

(±)-form [69814-97-7]

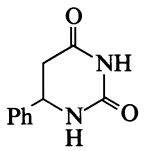
Solid. Mp 38°. Bp_{11} 171-172°, $Bp_{0.6}$ 115°.

Cromwell, N.H. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 4412 (*synth*)
Francotte, E. *et al*, *Helv. Chim. Acta*, 1987, **70**, 1569 (*resoln, abs config*)
Ballini, R. *et al*, *Synthesis*, 1987, 711 (*synth, ir, pmr*)

5,6-Dihydro-6-phenyl-2,4(1*H*, 3*H*)-pyrimidinedione, 9CI **D-80240**

6-Phenyldihydrouracil

[6300-95-4]



$C_{10}H_{10}N_2O_2$ M 190.201

(±)-*form*

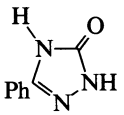
Cryst. Mp 216-218°.

Sandakhchiev, L.S. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1961, 72; *CA*, **56**, 2448.
Strekowski, L. *et al*, *Synthesis*, 1987, 579 (*synth, pmr*)

1,2-Dihydro-5-phenyl-3*H*-1,2,4-triazol-3-one, 9CI **D-80241**

5-Phenyl-$\Delta^{1,5}$*-1,2,4-triazolin-3-one*

[939-07-1]

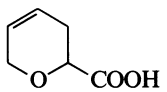


$C_8H_7N_3O$ M 161.163

Cryst. (butanol). Mp 323-324° (314-317°) dec.

Young, G. *et al*, *J. Chem. Soc.*, 1900, 224 (*synth*)
George, B. *et al*, *J. Org. Chem.*, 1976, **41**, 3233 (*synth, ir*)
Schantl, J.G. *et al*, *Synthesis*, 1987, 986 (*synth, ir, pmr*)

3,6-Dihydro-2*H*-pyran-2-carboxylic acid, 9CI **D-80242**



$C_6H_8O_3$ M 128.127

(±)-*form* [116233-54-6]

Oil. Bp_{10} 100°.

Et ester:

$C_8H_{12}O_3$ M 156.181

Liq. Bp_2 57-58°. d_4^{20} 1.07.

Amide:

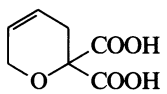
$C_6H_9NO_2$ M 127.143

Cryst. (diisopropyl ether). Mp 110-111°.

Arbuzov, A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1962, **142**, 341 (*ester*)
Mochalins, V.B. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1974, **44**, 2288 (*amide*)
Knapp, S. *et al*, *J. Org. Chem.*, 1988, **53**, 4773 (*synth, pmr, ir*)

3,6-Dihydro-2*H*-pyran-2,2-dicarboxylic acid, 9CI **D-80243**

[57668-92-5]



$C_7H_8O_5$ M 172.137

Golden oil.

Di-Et ester:

$C_{11}H_{16}O_5$ M 228.244

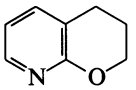
Oil. $Bp_{0.8}$ 100°.

Ruden, R.A. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 6892 (*synth*)
Bonjouklian, R. *et al*, *J. Org. Chem.*, 1977, **42**, 4095 (*synth*)
Knapp, S. *et al*, *J. Org. Chem.*, 1988, **53**, 4773 (*synth, pmr, ir*)

3,4-Dihydro-2*H*-pyrano[2,3-*b*]pyridine, 9CI **D-80244**

8-Azachroman

[26267-89-0]

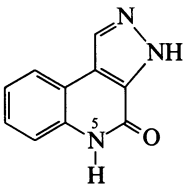


C_8H_9NO M 135.165

Pale yellow liq. Mp 30°. Bp_1 56°.

Sliwa, H., *Bull. Soc. Chim. Fr.*, 1970, 631 (*synth, ir, pmr*)
Taylor, E.C. *et al*, *Tetrahedron*, 1987, **43**, 5145 (*synth, ir, pmr, cmr*)

3,5-Dihydro-4*H*-pyrazolo[3,4-*c*]quinolin-4-one, 9CI **D-80245**



$C_{10}H_7N_3O$ M 185.185

N[5]*-Me:* [120757-42-8].

$C_{11}H_9N_3O$ M 199.212

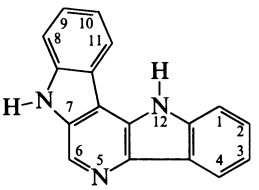
Pale yellow prisms (2-propanol). Mp >250°.

Ito, K. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1681 (*synth, pmr*)

7,12-Dihydropyrido[3,2-*b*:5,4-*b*′]diindole **D-80246**

*Pyrido[3,2-*b*:5,4-*b*′]diindole*

[98263-45-7]



$C_{17}H_{11}N_3$ M 257.294

7-Me: [116130-39-3].

$C_{18}H_{13}N_3$ M 271.321

Yellow solid. Mp >300°.

7-Me; B,HCl: [116130-40-6].

Solid. Mp >300°.

12-Me; B,HCl: [116130-42-8].

$C_{18}H_{13}N_3$ M 271.321

Mp >300°.

[116130-41-7, 116130-46-2]

Fukada, N. *et al*, *Tetrahedron Lett.*, 1985, **26**, 2139 (*synth*)
Trudell, M.L. *et al*, *J. Med. Chem.*, 1987, **30**, 456 (*synth*)
Trudell, M.L. *et al*, *J. Org. Chem.*, 1988, **53**, 4873 (*N*-Me, ms, pmr, ir)

3,4-Dihydro-2*H*-pyrrole, 9CI D-80247

Updated Entry replacing D-04055

1-Pyrroline

[5724-81-2]

C_4H_7N M 69.106

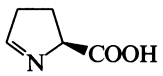
Stable in dil. soln., trimerises readily.

Poisel, H., *Monatsh. Chem.*, 1978, **109**, 925 (*synth, pmr*)
Bock, H. *et al*, *Chem. Ber.*, 1987, **120**, 1961 (*synth, pe, bibl*)
Guillemin, J.-C. *et al*, *Tetrahedron*, 1988, **44**, 4447 (*synth, pmr*)

3,4-Dihydro-2*H*-pyrrole-2-carboxylic acid, 9CI D-80248

1-Pyrroline-5-carboxylic acid, 8CI. 1,5-Didehydroproline

[2906-39-0]



(*S*)-*form*

$C_5H_7NO_2$ M 113.116

Dimerises in solution.

(*S*)-*form* [64199-88-8]

L-*form*

Intermed. in biosynth. and biodegradn. of L-proline.

(±)-*form* [23141-14-2]

Cryst. (H_2O). Mp 140-142° dec.

Et ester:

$C_7H_{11}NO_2$ M 141.169

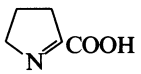
Liq. Bp_{17} 110°.

Vogel, H.J. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 109 (*synth, bibl*)
Osugi, K., *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1958, **78**, 1332; *CA*, **53**, 8109 (*synth, ester*)
Strecker, H.J. *et al*, *Methods Enzymol.*, *B*, 1971, **17**, 254 (*synth*)
Mezl, V.A. *et al*, *Anal. Biochem.*, 1976, **74**, 430 (*synth*)

3,4-Dihydro-2*H*-pyrrole-5-carboxylic acid, 9CI D-80249

1-Pyrroline-2-carboxylic acid, 8CI

[2139-03-9]



$C_5H_7NO_2$ M 113.116

Na salt: [72978-16-6].

Cryst. Mp 265° dec.

B,HBr: Cryst. (Et_2O). Mp 136° dec.

Me ester: [57224-14-3].

$C_6H_9NO_2$ M 127.143

Liq. $Bp_{0.13}$ 43°.

tert-*Butyl ester:* [74409-25-9].

$C_9H_{15}NO_2$ M 169.223

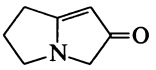
Liq. $Bp_{0.27}$ 43°.

Meister, A., *J. Biol. Chem.*, 1954, **206**, 577 (*synth*)
Macholan, L. *et al*, *Chem. Ber.*, 1963, **96**, 237 (*synth*)
Poisl, H. *et al*, *Chem. Ber.*, 1975, **108**, 2547 (*synth*)
Hänglen, J. *et al*, *Justus Liebigs Ann. Chem.*, 1981, 1073 (*esters, synth, pmr*)

2,3-Dihydro-1*H*-pyrrolizin-6(5*H*)-one, 9CI D-80250

*2,3,5,6-Tetrahydro-1*H*-pyrrolizin-6-one*

[97181-96-9]



C_7H_9NO M 123.154

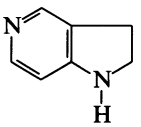
Oil. $Bp_{0.0006}$ 104°.

Pommelet, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5680 (*synth, ir, pmr, cmr, ms*)

2,3-Dihydro-1*H*-pyrrolo[3,2-*c*] pyridine, 9CI D-80251

5-Azaindoline

[23596-28-3]



$C_7H_8N_2$ M 120.154

Cryst (cyclohexane). Mp 102-103°.

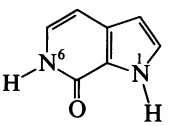
B,HCl: [5912-19-6].

Cryst. (EtOH/EtOAc). Mp 188-189°.

Yakhontov, L.N. *et al*, *J. Heterocycl. Chem. USSR* (*Engl. Transl.*), 1969, **5**, 410 (*synth, uv, ir, pmr*)

1,6-Dihydro-7*H*-pyrrolo[2,3-*c*]pyridin-7-one, 9CI D-80252

*1*H*-Pyrrolo[2,3-*c*]pyridin-7(6*H*)-one*



$C_7H_6N_2O$ M 134.137

6-Me: [116212-46-5].

$C_8H_8N_2O$ M 148.164

Clusters (toluene). Mp 190-192°.

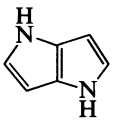
Dumas, D.J., *J. Org. Chem.*, 1988, **53**, 4650 (*synth, ir, pmr*)

1,4-Dihydropyrrolo[3,2-*b*]pyrrole, 9CI D-80253

Updated Entry replacing D-30286

*1,4-Dihydro-1,4-diazapentalene. Pyrrolo[3,2-*b*]pyrrole. 1,4-Diazapentalene*

[63156-05-8]



$C_6H_6N_2$ M 106.127

Needles (Me_2CO/hexane). Mp 123-124° dec. Unstable to air and acids.

1,4-Bis(methoxycarbonyl):

$C_{10}H_{10}N_2O_4$ M 222.200

Plates. Mp 163-164°.

1,4-Di-Me: [54724-95-7].

$C_8H_{10}N_2$ M 134.180

Mp 110°.

1,4-Diisopropyl: [117203-13-1].

$C_{12}H_{18}N_2$ M 190.288

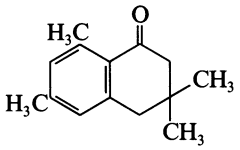
Bp_3 80°.

*1,4-Di-*tert*-butyl:* [117203-12-0].
$C_{14}H_{22}N_2$ M 218.341
Cryst.

Prinzbach, H. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1975, **14**, 347 (*deriv*)
Kumagai, T. *et al*, *Tetrahedron Lett.*, 1984, **25**, 5669 (*synth, ir, pmr, cmr, uv*)
tom Dieck, H. *et al*, *Chem. Ber.*, 1989, **122**, 129 (*synth, cryst struct, ir, raman, pmr, derivs*)

3,4-Dihydro-3,3,6,8-tetramethyl-1(2*H*)-napthalenone, 8CI, 9CI — D-80254

3,3,6,8-Tetramethyl-1-tetralone
[5409-55-2]

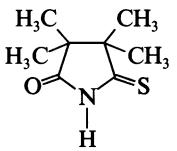


$C_{14}H_{18}O$ M 202.296
Condensation prod. of acetone. Cryst. (MeOH). Mp 56.5-57°. Bp 292-294°, Bp_{12} 146°.
2,4-Dinitrophenylhydrazone: [16695-83-3].
Red cryst. (EtOH/EtOAc). Mp 234°.
[38157-22-1]

Roger, A. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 3030 (*synth, uv, pmr, ir*)
Frank, H.-G. *et al*, *Justus Liebigs Ann. Chem.*, 1969, **724**, 94 (*synth*)
Riand, J., *Bull. Soc. Chim. Fr.*, 1975, 1339 (*ms*)
Haag, R. *et al*, *Helv. Chim. Acta*, 1977, **60**, 2595 (*pmr, props*)
Bertrand, J.A. *et al*, *J. Org. Chem.*, 1977, **42**, 1600 (*uv, pmr, ms*)

3,4-Dihydro-3,3,4,4-tetramethyl-5-thioxo-2(1*H*)pyrrolidinone — D-80255

2,2,3,3-Tetramethylmonothiosuccinimide

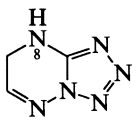


$C_8H_{13}NOS$ M 171.263
Pale yellow needles. Mp 102-105° subl.

Battersby, A.R. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1988, 1577 (*synth, ir, pmr, ms*)

7,8-Dihydrotetrazolo[1,5-*b*][1,2,4]triazine — D-80256

*1,7-Dihydrotetrazolo[1,5-*b*][1,2,4]triazine*
[117039-67-5]

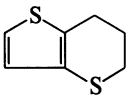


$C_3H_4N_6$ M 124.105
CAS no. refers to 1,7-dihydro. Cryst. (MeOH). Mp 161°.
8-Nitro: [117039-76-6].
$C_3H_3N_7O_2$ M 169.102
Cryst. Mp 124-126°. Dec. on recryst.

Willer, R. *et al*, *J. Org. Chem.*, 1988, **53**, 5371 (*synth, pmr, cmr*)

6,7-Dihydro-5*H*-thieno[3,2-*b*]thiopyran — D-80257

[7677-36-3]

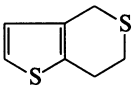


$C_7H_8S_2$ M 156.272
Oil. d_4^{20} 1.26. $Bp_{17.6}$ 136.5-137°.

Cagniant, P. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2172 (*synth*)

6,7-Dihydro-4*H*-thieno[3,2-*c*]thiopyran — D-80258

[16401-43-7]

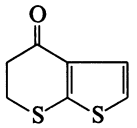


$C_7H_8S_2$ M 156.272
Strong smelling liq. d_4^{20} 1.25. Bp_{17} 141-142°.

Cagniant, P. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 2597 (*synth, uv, ir, pmr*)

2,3-Dihydro-4*H*-thieno[2,3-*b*]thiopyran-4-one — D-80259

[7675-04-9]

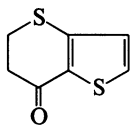


$C_7H_6OS_2$ M 170.256
Oil, slowly cryst. giving needles. Mp 61°. Bp_{15} 170°.
Oxime:
$C_7H_7NOS_2$ M 185.270
Cryst. (C_6H_6/pet. ether). Mp 128°.
Semicarbazone: Cryst. (EtOH). Mp 249.5°.
2,4-Dinitrophenylhydrazone: Red cryst. (C_6H_6/EtOH). Mp 260°.

Cagniant, P. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2172 (*synth*)
Ponticello, G.S. *et al*, *J. Org. Chem.*, 1988, **53**, 9 (*synth, pmr*)

5,6-Dihydro-7*H*-thieno[3,2-*b*]thiopyran-7-one — D-80260

[7677-33-0]



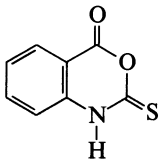
$C_7H_6OS_2$ M 170.256
Plates (EtOH aq.). Mp 71°. Bp_{14} 175°.
Oxime:
$C_7H_7NOS_2$ M 185.270
Cryst. (C_6H_6/pet. ether). Mp 178°.
Semicarbazone: Cryst. (EtOH). Mp 272°.
2,4-Dinitrophenylhydrazone: Red plates (EtOH/C_6H_6). Mp 210° and 245° (double Mp).

Cagniant, P. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2172 (*synth*)

1,2-Dihydro-2-thioxo-4*H*-3,1-benzoxazin-4-one, 9CI D-80261

2-Thioisatoic anhydride

[703-64-0]



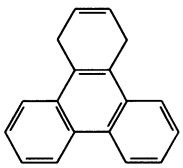
$C_8H_5NO_2S$ M 179.199

Cryst. (THF/CCl_4). Mp 239-241° (230-235°).

Marshall, J.R., *J. Chem. Soc.*, 1965, 938 (*synth, ir*)
Kricheldorf, H.R., *Chem. Ber.*, 1971, **104**, 3156 (*synth*)
Beam, C.F. *et al*, *J. Heterocycl. Chem.*, 1976, **13**, 421 (*synth*)

1,4-Dihydrotriphenylene D-80262

[39935-60-9]



$C_{18}H_{14}$ M 230.309

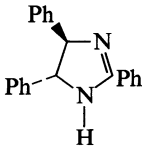
Cryst. (EtOH). Mp 203-204°.

Marcinow, Z. *et al*, *J. Org. Chem.*, 1988, **53**, 3603 (*synth, pmr*)

4,5-Dihydro-2,4,5-triphenyl-1*H*-imidazole, 9CI D-80263

2,4,5-Triphenyl-2-imidazoline, 8CI. 2,4,5-Triphenyldihydroglyoxaline

[37134-88-6]



(4*R**,5*R**)-*form*

$C_{21}H_{18}N_2$ M 298.387

(4R*,5R*)-form

(+)-trans-*form*
Mp 180°. $[\alpha]_D$ +46.3°.

(+)-*Tartrate salt:* Prisms (EtOH). Mp 175-176°. $[\alpha]_D^{13}$ +55.0° (c, 1.5 in EtOH).

(4S*,5S*)-form

(−)-trans-*form*
Mp 180°. $[\alpha]_D$ −46.9°.

(+)-*Tartrate salt:* Prisms (EtOAc). Mp 174-175°. $[\alpha]_D^{13}$ −67.1° (c, 1.5 in EtOH).

(4RS,5RS)-form [24427-33-6]

(±) trans-*form. Isoamarin*
Light tan cryst. (EtOH). Mp 198-201°.

1-Ac:
$C_{23}H_{20}N_2O$ M 340.424
Cryst. (pet. ether). Mp 114-116°.

1-Benzoyl:
$C_{28}H_{22}N_2O$ M 402.495
Cryst. (pet. ether). Mp 177-178°.

(4RS,5SR)-form [573-33-1]

(±)-cis-*form. Amarin*
Cryst. (C_6H_6/pet. ether). Mp 128-131°.

B,HCl: [42078-44-4].
Cryst. Mp 260-265°.

1-Ac: Cryst. (pet. ether). Mp 140-142°.

1-Benzoyl: Cryst. (pet. ether). Mp 179°.

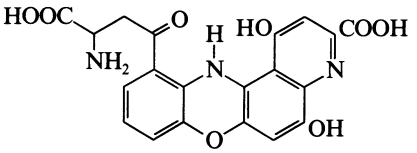
1-Benzyl:
$C_{28}H_{24}N_2$ M 388.511
Needles (EtOH). Mp 123-124°.

Claus, R. *et al*, *Chem. Ber.*, 1885, **18**, 3079 (*derivs*)
Snape, H.L., *J. Chem. Soc.*, 1900, **77**, 781 (*resoln*)
Williams, O.F. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 4464 (*synth*)
White, D.M. *et al*, *J. Org. Chem.*, 1964, **29**, 1926 (*ir*)
Hunter, D.H. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 6202 (*synth*)
Hunter, D.H. *et al*, *Can. J. Chem.*, 1972, **50**, 669 (*synth, pmr, deriv*)

Dihydroxanthommatin D-80264

*α-Amino-3-carboxydihydro-1-hydroxy-γ,5-dioxo-5*H*-pyrido[3,2-*a*]phenoxazine-11-butanoic acid, 9CI*

[25705-16-2]



$C_{20}H_{15}N_3O_8$ M 425.354

Found in eyes and skin of *Loligo vulgaris*, *Sepia officinalis* and other molluscs, also in heads of flies *Musca domestica* and bees *Apis mellifera*. The *O*-sulfate and *O*-glucoside prob. occur also.

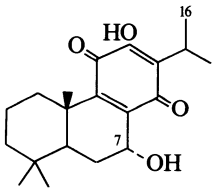
[121727-27-3]

Bolognese, A. *et al*, *Experientia*, 1974, **30**, 225.
Bolognese, A. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1247.

7,12-Dihydroxy-8,12-abietadiene-11,14-dione D-80265

Updated Entry replacing D-60304

7-Hydroxyroyleanone



$C_{20}H_{28}O_4$ M 332.439

7α-form [21887-01-4] ***Horminone***

Constit. of *Plectranthus* spp. Golden cryst. (MeOH aq.). Mp 178°. $[\alpha]_D$ −132° (c, 1.24 in $CHCl_3$).

*7-Ac: **7α-Acetoxyroyleanone.** 7-Acetylhorminone*
$C_{22}H_{30}O_5$ M 374.476
Isol. from whole plants of *Horminum pyrenaicum*, roots of *Salvia* spp. and leaf glands of *Coleus carnosus*.

*7-Formyl ester: **7-O-Formylhorminone***
$C_{21}H_{28}O_5$ M 360.449
Constit. of *Plectranthus sanguineus*. Yellow-orange cryst. (hexane). Mp 152.5-154°.

*7-Me ether: **7-O-Methylhorminone.** 7α-Methoxyroyleanone*
$C_{21}H_{30}O_4$ M 346.466
Constit. of *Lepechinia bullata*. Yellow cryst. ($CHCl_3$). Mp 126-128°.

*12-Ac, 16-acetoxy: 16-Acetoxy-12-*O*-acetylhorminone*
$C_{24}H_{32}O_7$ M 432.513
Constit. of *R. lophanthoides*. Yellow needles. Mp 158°.

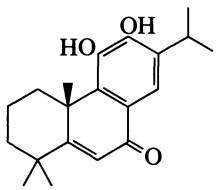
7β-form [21764-41-0] ***Taxoquinone***
Isol. from *Taxodium distichum*. Mp 214°. $[\alpha]_D^{25}$ +240° (c, 1.4 in $CHCl_3$).

Kupchan, S.M. *et al*, *J. Org. Chem.*, 1969, **34**, 3912 (*isol*)
Hensch, M. *et al*, *Helv. Chim. Acta*, 1975, **58**, 1921 (*isol*)
Bhat, S.V. *et al*, *Tetrahedron*, 1975, **31**, 1001 (*isol, deriv*)
Matsumoto, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 1459 (*synth*)
Hueso-Rodriguez, J.A. *et al*, *Phytochemistry*, 1983, **22**, 2005 (*isol, derivs*)
Matloubi-Moghadam, F. *et al*, *Helv. Chim. Acta*, 1987, **70**, 975 (*isol, deriv*)
Jonathan, L.T. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 571 (*isol, deriv, pmr, cmr*)

11,12-Dihydroxy-5,8,11,13-abietatetraen-7-one D-80266

Salvinolone

[120278-22-0]



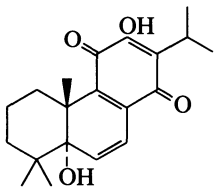
$C_{20}H_{26}O_3$ M 314.424
Constit. of *Salvia prionitis*. Cryst. Mp 253-254°. $[\alpha]_D$ +35.8° (c, 0.12 in MeOH).

Lin, L.-Z. *et al*, *Phytochemistry*, 1989, **28**, 177.

5,12-Dihydroxy-6,8,12-abietatriene-11,14-dione D-80267

Hypargenin F

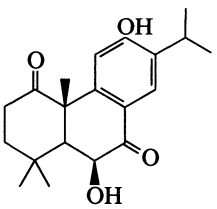
[119767-16-7]



$C_{20}H_{26}O_4$ M 330.423
Constit. of *Salvia hypargeia*. Antibacterial agent. Dark red amorph. solid.

Ulubelen, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1178 (*isol, pmr, cmr*)

6,12-Dihydroxy-8,11,13-abietatriene-1,7-dione D-80268



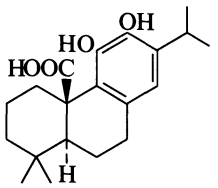
$C_{20}H_{26}O_4$ M 330.423
6β-form [119767-12-3] ***Hypargenin A***
Constit. of *Salvia hypargeia*. Antibacterial agent. Dark yellow amorph. solid.

Ulubelen, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1178 (*isol, pmr,*)

11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid D-80269

Carnosic acid. *Deoxypicrosalvinic acid*

[3650-09-7]



$C_{20}H_{28}O_4$ M 332.439
Isol. from *Salvia officinalis* and *Rosmarinus officinalis*. Cryst. (hexane). Mp 185-190° dec. $[\alpha]_D^{23}$ +191° (c, 1.07 in MeOH).

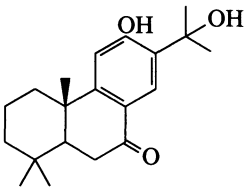
Di-Ac: Needles (hexane). Mp 212-217°. $[\alpha]_D^{22}$ +139° (c, 1.15 in $CHCl_3$).

Linde, H. *et al*, *Helv. Chim. Acta*, 1964, **47**, 1234 (*isol, uv, ir, pmr*)
Wenkert, E. *et al*, *J. Org. Chem.*, 1965, **30**, 2931 (*isol, ir, pmr, config*)
Meyer, W.L. *et al*, *Tetrahedron Lett.*, 1966, 4261 (*synth*)

12,15-Dihydroxy-8,11,13-abietatrien-7-one D-80270

Hypargenin B

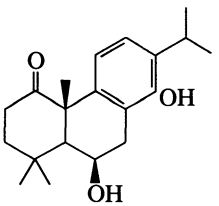
[119767-13-4]



$C_{20}H_{28}O_3$ M 316.439
Constit. of *Salvia hypargeia*. Antibacterial agent. Orange amorph. solid.

Ulubelen, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1178 (*isol, pmr*)

6,14-Dihydroxy-8,11,13-abietatrien-1-one D-80271



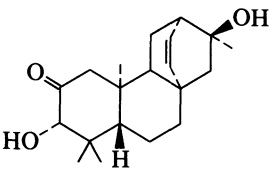
$C_{20}H_{28}O_3$ M 316.439
6β-form [119767-15-6] ***Hypargenin E***
Constit. of *Salvia hypargeia*. Amorph.

Ulubelen, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1178 (*isol, pmr*)

ent-3β,16α-Dihydroxy-13-atisen-2-one D-80272

Yucalexin A-19

[119642-83-0]

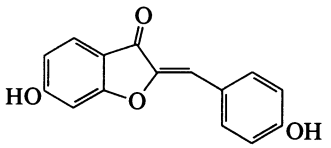


$C_{20}H_{30}O_3$ M 318.455
Constit. of cassava roots (*Manihot esculenta*). $[\alpha]_D^{23}$ +8.28° (c, 0.35 in $CHCl_3$).

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

4′,6-Dihydroxyaurone D-80273

6-Hydroxy-2-[(4-hydroxyphenyl)methylene]-3(2H)-benzofuranone, 9CI. 6-Hydroxy-2-(p-hydroxybenzylidene)-3(2H)benzofuranone, 8CI. ***Hispidol***



$C_{15}H_{10}O_4$ M 254.242

(Z)-form [5786-54-9]
Isol. from seedlings of *Glycine max* (*Soja hispida*) and from *Lygos raetam*. Yellow needles (EtOH aq.). Mp 288° dec.

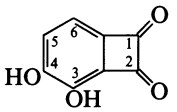
Di-Ac: Pale-yellow needles (MeOH/AcOH). Mp 162-163°.

6-O-β-D-Glucopyranosyl: [20550-08-7].
$C_{21}H_{20}O_9$ M 416.384
Isol. from seedlings of *G. max* and from *L. raetam*. Yellow cryst. (H_2O). Mp 211-212° (191-192°).

Geissman, T.A. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 832 (*synth, uv*)
Wong, E., *Phytochemistry*, 1966, **5**, 463 (*isol*)
Farkas, L. *et al*, *Tetrahedron*, 1968, **24**, 4213 (*synth*)
Huke, M. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1969, **302**, 401, 423 (*uv, pmr*)
El Sherbeiny, A.E.A. *et al*, *Planta Med.*, 1978, **34**, 335 (*isol*)

3,4-Dihydroxybenzocyclobutene-1,2-dione D-80274

2,3-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione



$C_8H_4O_4$ M 164.117

Di-Me ether: [118112-21-3]. *3,4-Dimethoxbenzocyclobutene-1,2-dione*
$C_{10}H_8O_4$ M 192.171
Cryst. (H_2O). Mp 146°.

Methylene ether: [118112-23-5]. *3,4-Methylenedioxybenzocyclobutene-1,2-dione*
$C_9H_4O_4$ M 176.128
Cryst. (Me_2CO aq.). Mp 164-166°.

Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, ir, pmr, cmr*)

3,5-Dihydroxybenzocyclobutene-1,2-dione D-80275

2,4-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione

$C_8H_4O_4$ M 164.117

Di-Me ether: [118112-22-4]. *3,5-Dimethoxybenzocyclobutene-1,2-dione*
$C_{10}H_8O_4$ M 192.171
Cryst. (hexane). Mp 147-148°.

Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, ir, pmr, cmr*)

3,6-Dihydroxybenzocyclobutene-1,2-dione D-80276

2,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione

[75833-49-7]

$C_8H_4O_4$ M 164.117
Cryst. (H_2O). Mp 225-228°. pK_{a1} 5.3 (25°), pK_{a2} 9.3.

Di-Me ether: [75833-47-5]. *3,6-Dimethoxybenzocyclobutene-1,2-dione*
$C_{10}H_8O_4$ M 192.171
Yellow plates (cyclohexane). Mp 190-192°.

Abou-Teim, I. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1980, 1841 (*synth, deriv, uv, ir, pmr*)
Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, deriv, ir, pmr, cmr*)

4,5-Dihydroxybenzocyclobutene-1,2-dione D-80277

3,4-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione

[41737-30-8]

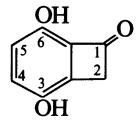
$C_8H_4O_4$ M 164.117
Benzologue of squaric acid. Yellow prisms (H_2O). Mp 243-245° dec. pK_{a1} 4.48 (20°), pK_{a2} 8.05.

Di-Me ether: [41634-27-9]. *4,5-Dimethoxybenzocyclobutene-1,2-dione*
$C_{10}H_8O_4$ M 192.171
Needles (cyclohexane). Mp 222-223°.

Abou-Teim, O. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1841 (*synth, uv, ir, pmr*)

3,6-Dihydroxybenzocyclobuten-1-one D-80278

Updated Entry replacing D-20333
2,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one



$C_8H_6O_3$ M 150.134

Di-Me ether: [75833-45-3]. *3,6-Dimethoxybenzocyclobuten-1-one. 2,5-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-one*
$C_{10}H_{10}O_3$ M 178.187
Cryst. (pet. ether). Mp 107-108°.

McOmie, J.F.W. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1841 (*synth, ir, pmr*)
Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, ir, pmr, cmr*)

4,5-Dihydroxybenzocyclobuten-1-one D-80279

Updated Entry replacing D-20334
3,4-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one

$C_8H_6O_3$ M 150.134

Di-Me ether: [55171-76-1]. *4,5-Dimethoxybenzocyclobuten-1-one. 3,4-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-one, 9CI*
$C_{10}H_{10}O_3$ M 178.187
Plates. Mp 142-143°. $Bp_{0.05}$ 140° subl.

Kametani, T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1974, 1712 (*synth, ir, uv, pmr*)

4,6-Dihydroxybenzocyclobuten-1-one D-80280

3,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one

$C_8H_6O_3$ M 150.134

Di-Me ether: [118112-18-8]. *4,6-Dimethoxybenzocyclobuten-1-one*
$C_{10}H_{10}O_3$ M 178.187

Cryst. (H_2O). Mp 51-52°.

Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, ir, pmr, cmr*)

5,6-Dihydroxybenzocyclobuten-1-one D-80281

Updated Entry replacing D-20335

4,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one

$C_8H_6O_3$ M 150.134

Di-Me ether: [81447-58-7]. *5,6-Dimethoxybenzocyclobuten-1-one. 4,5-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-one, 9CI*

$C_{10}H_{10}O_3$ M 178.187

Cryst. (pet. ether). Mp 86-87°.

Stevens, R.V. *et al*, *J. Org. Chem.*, 1982, **47**, 2393 (*synth, ir, pmr*)

Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, ir, pmr, cmr*)

5,7-Dihydroxy-2*H*-1-benzopyran-2-one, 9CI D-80282

Updated Entry replacing D-04285

5,7-Dihydroxycoumarin

[2732-18-5]

$C_9H_6O_4$ M 178.144

Found in *Rumex conglomeratus*. Prisms (AcOH aq.), yellow needles (H_2O). Mp 285-286°.

▷ Exp. carcinogen.

Di-Ac: [21524-17-4].

$C_{13}H_{10}O_6$ M 262.218

Prisms (EtOH). Mp 140°.

Di-Me ether: [487-06-9]. *5,7-Dimethoxy-2H-1-benzopyran-2-one. 5,7-Dimethoxycoumarin.* ***Citropten.*** *Limettin*

$C_{11}H_{10}O_4$ M 206.198

Found in lime and bergamot oils, *Eriostema obovalis, Xanthoxylum inerme* and *Glycosmis cyanocarpa*. Prisms (MeOH). Mp 147°. Fluorescent in EtOH.

O^5-*(2-Propenyl)*: [23053-60-3]. *7-Hydroxy-5-(2-propenyloxy)-4H-1-benzopyran-2-one, 9CI. 5-Allyloxy-7-hydroxycoumarin.* ***Lacoumarin***

$C_{12}H_{10}O_4$ M 218.209

Constit. of *Lawsonia inermis*. Mp 162-164°.

O^5-*(3-Methyl-2-butenyl)*, O^7-*Me:*

$C_{15}H_{16}O_4$ M 260.289

Isol. from *Citrus limon*. Mp 90-92°.

O^5-*(3,7-Dimethyl-2,6-octadienyl)*, O^7-*Me:*

$C_{20}H_{24}O_4$ M 328.407

Isol. from *C. aurantifolia*. Mp 86-87°.

O^5-*(6-Hydroxy-3,7-dimethyl-2,6-octadienyl)*, O^7-*Me:*

$C_{20}H_{24}O_5$ M 344.407

Isol. from *C. aurantifolia*.

O^7-*(3-Methyl-2-butenyl)*: ***Anisocoumarin B***

$C_{14}H_{14}O_4$ M 246.262

Constit. of *Clausena anisata*. Granules. Mp 94-95°.

Heyes, R.G. *et al*, *J. Chem. Soc.*, 1936, 1831 (*synth*)

Gerphagnon, M.C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1958, **246**, 1201 (*uv*)

Crombie, L. *et al*, *J. Chem. Soc. C*, 1971, 788 (*synth, ir, pmr, ms*)

Talapatra, B. *et al*, *Indian J. Chem.*, 1975, **13**, 835 (*isol, deriv*)

Günther, D.H. *et al*, *Org. Magn. Reson.*, 1975, **7**, 339 (*cmr, deriv*)

Bhardwaj, D.K. *et al*, *Phytochemistry*, 1976, **15**, 1789 (*Lacoumarin*)

Gray, A.I. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1978, 391 (*pmr*)

Joseph-Nathan, P. *et al*, *J. Heterocycl. Chem.*, 1984, **21**, 1141 (*pmr, deriv*)

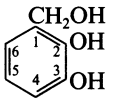
Ngadjai, B.J. *et al*, *Phytochemistry*, 1989, **28**, 585 (*Anisocoumarin B*)

Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 594.

2,3-Dihydroxybenzyl alcohol D-80283

3-(Hydroxymethyl)-1,2-benzenediol, 9CI

[14235-77-9]



$C_7H_8O_3$ M 140.138

O^2-*β-D-Glucoside:* [20331-85-5]. ***Idesin***

$C_{13}H_{18}O_8$ M 302.280

Isol.from leaves of *Idesia polycarpa*. Mp 98-100°.

Kubota, T. *et al*, *Bot. Mag.*, 1966, **79**, 770; *CA*, **68**, 49982 (*Idesin*)

3,4-Dihydroxybenzyl alcohol, 8CI D-80284

Updated Entry replacing D-04308

3,4-Dihydroxybenzenemethanol, 9CI. α,3,4-Trihydroxytoluene. Protocatechuyl alcohol. 4-Hydroxymethyl-1,2-benzenediol

[3897-89-0]

$C_7H_8O_3$ M 140.138

Prisms (H_2O). Mp 137-138°. Highly air-sensitive.

Tri-Ac:

$C_{13}H_{14}O_6$ M 266.250

$Bp_{0.05}$ 143-147°.

4-O-β-D-Gluocopyranoside: [20300-53-2]. ***Calleryanin***

$C_{13}H_{18}O_8$ M 302.280

Isol. from leaves of *Pyrus calleryana*. Occurs partly as various aromatic esters, not fully characterised.

O^4-*(6-O-Benzoyl-β-D-glucopyranoside)*: [41942-94-3]. ***Lacticolorin***

$C_{10}H_{22}O_9$ M 286.278

Isol. from leaves of *Protea lacticolor*. Cryst. (H_2O). Mp 192-195°. $[\alpha]_D$ −58° (c, 0.59 in MeOH).

3-Me ether: [498-00-0]. *4-Hydroxy-3-methoxybenzenemethanol, 9CI. α,4-Dihydroxy-3-methoxytoluene. Vanillyl alcohol*

$C_8H_{10}O_3$ M 154.165

Cryst. (H_2O). Mp 114-115°.

4-Me ether: [4383-06-6]. *3-Hydroxy-4-methoxybenzenemethanol, 9CI. 3-Hydroxy-4-methoxybenzyl alcohol, 8CI. Isovanillyl alcohol*

Cryst. (toluene). Mp 131-132°.

Rosenmund, K.W. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1926, **264**, 458.

Pearl, I.A., *J. Org. Chem.*, 1947, **12**, 79 (*deriv*)

Cook, P.L. *et al*, *J. Org. Chem.*, 1962, **27**, 3873 (*deriv*)

Kaemmerer, H. *et al*, *Makromol. Chem.*, 1963, **67**, 167 (*synth*)

Challice, J.S. *et al*, *Phytochemistry*, 1968, **7**, 119 (*Calleryanin*)

Perold, G.W. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 638 (*Lacticolorin*)

Danishevsky, S. *et al*, *J. Org. Chem.*, 1976, **41**, 1081 (*deriv*)

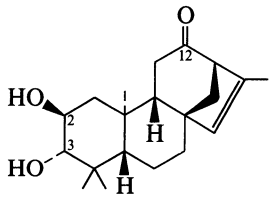
Krohn, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1977, 1186 (*Lacticolorin*)

Becher, H.D. *et al*, *J. Org. Chem.*, 1980, **45**, 1596 (*deriv*)

ent-2α,3β-Dihydroxy-15-beyeren-12-one D-80285

Yucalexin B-22

[119626-55-0]



$C_{20}H_{30}O_3$ M 318.455
Constit. of cassava roots (*Manihot esculenta*).

2-Ketone: [35470-61-2]. ent-3*β-Hydroxy*-15-*beyerene*-2,12-*dione*. ***Yucalexin B-9***
$C_{20}H_{28}O_3$ M 316.439
Constit. of *M. esculenta*. $[\alpha]_D^{23}$ −73.9° (c, 0.83 in $CHCl_3$).

2,3-Diketone: [50719-31-8]. ent-15-*Beyerene*-2,3,12-*trione*. ent-2-*Hydroxy*-1,15-*beyeradiene*-3,12-*dione*. ***Yucalexin B-5***
$C_{20}H_{26}O_3$ M 314.424
Constit. of *M. esculenta*. Exists as an enol form.

2-Deoxy: [119626-51-6]. ent-3*β-Hydroxy*-15-*beyeren*-12-*one*. ***Yucalexin B-14***
$C_{20}H_{30}O_2$ M 302.456
Constit. of *M. esculenta*.

2-Deoxy, 3-ketone: [88048-00-4]. ent-15-*Beyerene*-3,12-*dione*. ***Yucalexin B-6***
$C_{20}H_{28}O_2$ M 300.440
Constit. of *M. esculenta*.

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

ent-3β,12α-Dihydroxy-15-beyeren-2-one D-80286

Yucalexin B-20

[119679-04-8]

$C_{20}H_{30}O_3$ M 318.455
Constit. of cassava roots (*Manihot esculenta*).

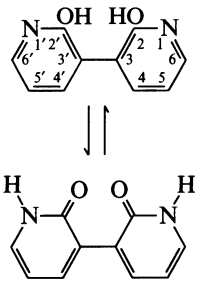
12-Epimer: [119626-53-8]. ent-3*β*,12*β-Dihydroxy*-15-*beyeren*-2-*one*. ***Yucalexin B-18***
$C_{20}H_{30}O_3$ M 318.455
Constit. of *M. esculenta*. $[\alpha]_D^{26}$ −9.4° (c, 0.17 in $CHCl_3$).

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

2,2′-Dihydroxy-3,3′-bipyridine D-80287

[*3,3′-Bipyridine*]-*2,2′*(*1*H,*1′*H)-*dione*, *9CI*. [*3,3′-Bipyridine*]-*2,2′-diol*. *3,3′-Bi-2-pyridone*

[97033-24-4]



$C_{10}H_8N_2O_2$ M 188.185
Pyridone tautomers prob. predominate where feasible in this series. Entries are given under the dihydroxydipyridine names for ease of presentation.
Cryst. Mp >300°.

Di-Me ether: [95881-80-4]. *2,2′-Dimethoxy*-3,3′-*bipyridine*, *9CI*
$C_{12}H_{12}N_2O_2$ M 216.239
Mp 117-118°.

Becalski, A. *et al*, *Bull. Pol. Acad. Sci., Chem.*, 1984, **32**, 105 (*synth, ir, ms, pmr*)
Tiecco, M. *et al*, *Synthesis*, 1984, 736 (*synth, deriv, pmr*)
Kaczmarek, L., *Pol. J. Chem.* (*Rocz. Chem.*), 1985, **59**, 1141 (*synth*)

2,2′-Dihydroxy-4,4′-bipyridine D-80288

[*4,4′-Bipyridine*]-*2,2′-diol*. [*4,4′-Bipyridine*]-*2,2′*(*1*H,*1′*H)-*dione*. *4,4′-Bi-2-pyridone*

[58426-03-2]

$C_{10}H_8N_2O_2$ M 188.185
Cryst. (H_2O). Mp >300°.

Abramovitch, R.A. *et al*, *J. Org. Chem.*, 1976, **41**, 1717 (*synth, ir, ms, pmr*)

2,4′-Dihydroxy-1,1′-bipyridine D-80289

[*1,1′*(2H,*4′*H)-*Bipyridine*]-*2,4′-dione*, *9CI*

[68304-41-6]

$C_{10}H_8N_2O_2$ M 188.185
Prisms (EtOH). Mp 233-236°.

B, HCl: [68304-44-9].
Prisms (EtOH). Mp 210-212°.

Katritzky, A.R. *et al*, *Pak. J. Sci. Ind. Res.*, 1978, **21**, 1 (*synth, ir, pmr, uv*)
Afridi, A.S. *et al*, *J. Chem. Soc. Pak.*, 1982, **4**, 55 (*ms*)

3,3′-Dihydroxy-2,2′-bipyridine D-80290

[*2,2′-Bipyridine*]-*3,3′-diol*, *9CI*

[36145-03-6]

$C_{10}H_8N_2O_2$ M 188.185
Cryst. by subl. Mp 196° (188-190°).

Mono-Me ether: [87385-13-5]. *3-Hydroxy-3′-methoxy*-2,2′-*bipyridine*
$C_{11}H_{10}N_2O_2$ M 202.212
Yellow cryst. ($CHCl_3$/pet. ether). Mp 85°.

Di-Me ether: [93560-59-9]. *3,3′-Dimethoxy*-2,2′-*bipyridine*
$C_{12}H_{12}N_2O_2$ M 216.239
Cryst. (CCl_4). Mp 138°.

Siemanowski, W. *et al*, *Justus Liebigs Ann. Chem.*, 1984, 1731 (*synth, deriv, pmr*)
Tiecco, M. *et al*, *Synthesis*, 1984, 736 (*deriv, synth, pmr*)
Tiecco, M. *et al*, *Tetrahedron*, 1986, **42**, 1475 (*synth, pmr, cmr*)

3,3′-Dihydroxy-4,4′-bipyridine D-80291

4,4′-Bipyridine-3,3′-diol

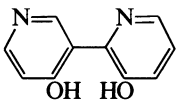
$C_{10}H_8N_2O_2$ M 188.185
Cryst. (MeOH). Mp 190-191°.

Ziyaev, A.A. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1964, **34**, 349 (*synth*)

3,4′-Dihydroxy-2,3′-bipyridine D-80292

[*2,3′-Bipyridine*]-*3,4′-diol*, *9CI*

[89945-98-2]



$C_{10}H_8N_2O_2$ M 188.185

Alkaloid from the timber of *Broussonetia zeylanica* (Moraceae). Deep-yellow cryst. ($CHCl_3$). Mp 171-173°, Mp 223-224°. Struct. of the nat. prod. in doubt; authentic synthetic material (Mp 171-173°) is not identical with the alkaloid assigned this struct.

Di-Ac: [89945-99-3].
Cryst. (C_6H_6/pet. ether). Mp 160-161°.

Gunatilaka, A.A.L. *et al*, *Phytochemistry*, 1983, **22**, 2847 (*isol, uv, ir, pmr, cmr, ms, struct*)
Dehmlow, E.V. *et al*, *Justus Liebigs Ann. Chem.*, 1987, 1123 (*synth, uv, ir, pmr, cmr*)

4,4′-Dihydroxy-1,1′-bipyridine D-80293

[1,1′(4H,4′H)-Bipyridine]-4,4′-dione, 9CI. 1,1′-Bipyridine-4,4′-diol. 1,1′-Bi-4-pyridone

[68304-42-7]

$C_{10}H_8N_2O_2$ M 188.185
Prisms (EtOH). Mp 205-210° dec.

B,HCl: [68304-43-8].
Prisms (EtOH). Mp 210-230° dec.

Katritzky, A.R. *et al*, *Pak. J. Sci. Ind. Res.*, 1978, **21**, 1 (*synth, ir, pmr, uv*)
Afridi, A.S. *et al*, *J. Chem. Soc. Pak.*, 1982, **4**, 55 (*ms*)

4,4′-Dihydroxy-2,2′-bipyridine D-80294

[2,2′-Bipyridine]-4,4′-diol. [2,2′-Bipyridine]-4,4′(1H,1′H)-dione. 2,2′-Bi-4-pyridone

$C_{10}H_8N_2O_2$ M 188.185
Cryst. (H_2O). Mp 342-343°. Forms a hemihydrate.

1,1′-Dioxide:
$C_{10}H_8N_2O_4$ M 220.184
Mp 308° dec.

Di-Me ether: [17217-57-1]. *4,4′-Dimethoxy-2,2′-bipyridine, 9CI*
$C_{12}H_{12}N_2O_2$ M 216.239
Cryst. (EtOH). Mp 170-172°.

Di-Me ether, 1,1′-dioxide: [84175-10-0].
$C_{12}H_{12}N_2O_4$ M 248.238
Cryst. Mp 229° dec.

Di-Me ether, 1,1′-dioxide, picrate: Cryst. Mp 190.5-192°.

Haginiwa, J., *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1955, **75**, 733 (*dioxide*)
Case, F.H., *J. Org. Chem.*, 1962, **27**, 640 (*synth*)
Stoesser, R. *et al*, *Z. Chem.*, 1978, **18**, 187 (*esr*)
Wenkert, D. *et al*, *J. Org. Chem.*, 1983, **48**, 283 (*synth derivs, pmr, ir, uv*)
Connor, J.A. *et al*, *J. Organomet. Chem.*, 1985, **282**, 349 (*pmr, deriv*)

4,4′-Dihydroxy-3,3′-bipyridine D-80295

[3,3′-Bipyridine]-4,4′-diol, 9CI. [3,3′-Bipyridine]-4,4′(1H,1′H)-dione, 9CI. 3,3′-Bi-4-pyridone

[27353-34-0]

$C_{10}H_8N_2O_2$ M 188.185
Needles.

[109324-77-8]

Kosuge, T. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 1068 (*synth, ir, uv*)
Kaczmarek, L., *Pol. J. Chem.* (*Rocz. Chem.*), 1985, **59**, 1141 (*synth*)

4,6-Dihydroxy-2,2′-bipyridine D-80296

[2,2′-Bipyridine]-4,6-diol

$C_{10}H_8N_2O$ M 172.186

O^4-*Me:* [14759-78-5]. *4-Methoxy-2,2′-bipyridin-6-ol, 8CI. 6-Hydroxy-4-methoxy-2,2′-bipyridine*
$C_{11}H_{10}N_2O_2$ M 202.212
Needles (C_6H_6). Mp 172.5°.

Divekar, P.V. *et al*, *Can. J. Chem.*, 1967, **45**, 1215 (*synth, ir, uv*)

5,5′-Dihydroxy-2,2′-bipyridine D-80297

2,2′-Bipyridine-5,5′-diol

$C_{10}H_8N_2O_2$ M 188.185
Cryst. Mp 250°.

[39858-87-2]

Otroshchenko, O.S. *et al*, *CA*, 1964, **63**, 4248e (*synth*)

5,5′-Dihydroxy-3,3′-bipyridine D-80298

3,3′-Bipyridine-5,5′-diol

$C_{10}H_8N_2O_2$ M 188.185

Di-Me ether: [95881-81-5]. *5,5′-Dimethoxy-3,3′-bipyridine, 9CI*
$C_{12}H_{12}N_2O_2$ M 216.239
Mp 161-162°.

Tiecco, M. *et al*, *Synthesis*, 1984, 736 (*synth, pmr, deriv*)

6,6′-Dihydroxy-2,2′-bipyridine D-80299

[2,2′-Bipyridine]-6,6′-(1H,1′H)-dione, 9CI. 2,2′-Bipyridine-6,6′-diol. 6,6′-Bi-2-pyridone

$C_{10}H_8N_2O_2$ M 188.185
Sesquihydrate. Mp 325-326° dec.

Di-Ac:
$C_{14}H_{12}N_2O_4$ M 272.260
Mp 175-176° dec.

Di-Me ether: [39858-88-3]. *6,6′-Dimethoxy-2,2′-bipyridine, 9CI*
$C_{12}H_{12}N_2O_2$ M 216.239
Mp 118°.

Dihydrazone: [53301-38-5].
$C_{10}H_{12}N_6$ M 216.245
Yellow needles (H_2O). Mp 208°.

Murase, I., *Nippon Kagaku Zasshi* (*Jpn. J. Chem.*), 1956, **77**, 682; *CA*, **52**, 91006 (*synth*)
Lewis, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 734 (*hydrazone*)
Tiecco, M. *et al*, *Synthesis*, 1984, 736 (*synth, deriv, pmr*)
Vanderesse, R. *et al*, *Tetrahedron Lett.*, 1986, **27**, 5483 (*synth, deriv*)

6,6′-Dihydroxy-3,3′-bipyridine D-80300

3,3′-Bipyridine-6,6′-diol. [3,3′-Bipyridine]-6,6′(1H,1′H)-dione. 5,5′-Bi-2-pyridone

$C_{10}H_8N_2O_2$ M 188.185

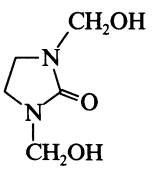
Di-Me ether: [95881-82-6]. *6,6′-Dimethoxy-3,3′-bipyridine, 9CI*
$C_{12}H_{12}N_2O_2$ M 216.239
Mp 104-105°.

Tiecco, M. *et al*, *Synthesis*, 1984, 736 (*synth, pmr, deriv*)

4,5-Dihydroxy-1,3-bis(hydroxymethyl)-2-imidazolidinone, 9CI D-80301

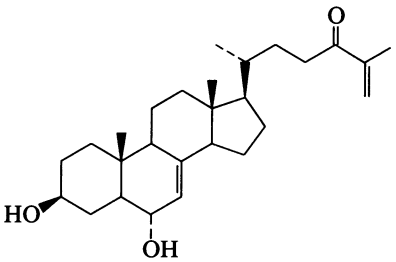
Dihydroxydimethylethyleneurea. Dimethyloldihydroxyethyleneurea. Dihydroxy DMEU. DMDHEU

[1854-26-8]



$C_5H_{10}N_2O_5$ M 178.144
Cross-linking agent. Textile-finishing agent, especially for cotton garments. Hygroscopic cryst.
U.K. Pat., 720 386, (1954); *CA*, **49**, 9326i (*manuf*)
Soignet, D.M. *et al*, *Appl. Spectrosc.*, 1970, **24**, 272 (*pmr*)
Beck, K.R. *et al*, *J. Chromatogr.*, 1980, **190**, 226 (*chromatog*)
Andrews, B.A.K., *J. Chromatogr.*, 1984, **288**, 101 (*cmr, hplc*)
Hermanns, K. *et al*, *Ind. Eng. Chem. Prod. Res. Dev.*, 1986, **25**, 469 (*cmr, bibl*)
Eur. Pat., 221 537, (1987); *CA*, **107**, 238841c (*manuf*)

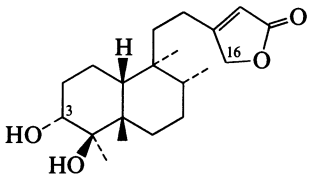
3,6-Dihydroxy-7,25-cholestadien-24-one D-80302



$C_{27}H_{42}O_3$ M 414.627
(3β,5α,6α)-form
Constit. of *Spongionella gracilis*.
Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol, pmr*)

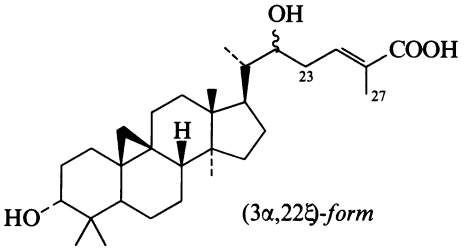
ent-3β,4α-Dihydroxy-13-cleroden-15,16-olide D-80303

[118173-00-5]



$C_{20}H_{32}O_4$ M 336.470
Constit. of *Ageratina saltillensis*.
3-Me ether: [118173-01-6]. **ent-*4α-Hydroxy-3β-methoxy-13-cleroden-15,16-olide***
$C_{21}H_{34}O_4$ M 350.497
Constit. of *A. saltillensis*.
3-Ketone: [118173-02-7]. **ent-*4α-Hydroxy-3-oxo-13-cleroden-15,16-olide***
$C_{20}H_{30}O_4$ M 334.455
Constit. of *A. saltillensis*.
16ξ-Hydroxy: [118172-99-9]. **ent-*3β,4α,16ξ-Trihydroxy-13-cleroden-15,16-olide***
$C_{20}H_{32}O_5$ M 352.470
Constit. of *A. saltillensis*.
Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187.

3,22-Dihydroxy-24-cycloarten-26-oic acid D-80304



$C_{30}H_{48}O_4$ M 472.707
(3α,22ξ)-form
Constit. of *Mangifera indica*. Cryst. ($CHCl_3$/MeOH). Mp 218-220°. $[\alpha]_D^{30}$ +27.5° (c, 0.8 in $CHCl_3$).
(3β,22ξ)-form
Constit. of *M. indica*.
Anjaneyulu, V. *et al*, *Phytochemistry*, 1989, **28**, 1471.

3,23-Dihydroxy-24-cycloarten-26-oic acid D-80305

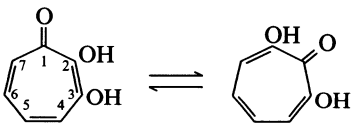
$C_{30}H_{48}O_4$ M 472.707
(3β,23ξ)-form
Constit. of *Mangifera indica*.
Anjaneyulu, V. *et al*, *Phytochemistry*, 1989, **28**, 1471.

3,27-Dihydroxy-24-cycloarten-26-oic acid D-80306

$C_{30}H_{48}O_4$ M 472.707
3α-form
Constit. of *Mangifera indica*. Cryst. (C_6H_6/EtOAc). Mp 205-207°. $[\alpha]_D^{30}$ +21.5° (c, 0.8 in $CHCl_3$).
Anjaneyulu, V. *et al*, *Phytochemistry*, 1989, **28**, 1471.

2,3-Dihydroxy-2,4,6-cycloheptatrien-1-one D-80307

2,3-Dihydroxytropone. 3-Hydroxytropolone. 2,7-Dihydroxytropone. 7-Hydroxytropolone
[34777-04-3]



$C_7H_6O_3$ M 138.123
Prod. by a *Pseudomonas* strain. Shows antibacterial activity. Mp 143-144° (139°).
Korth, H. *et al*, *Z. Naturforsch.*, *C*, 1981, **36**, 728 (*isol, ms, uv, pmr*)
Takeshita, H. *et al*, *Synthesis*, 1986, 578 (*synth, cmr, bibl*)

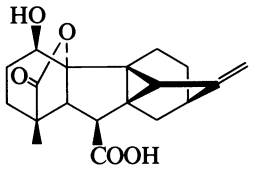
2,4-Dihydroxy-2,4,6-cycloheptatrien-1-one D-80308

2,4-Dihydroxytropone. 4-Hydroxytropolone. 2,6-Dihydroxytropone. 6-Hydroxytropolone
[7009-19-0]
$C_7H_6O_3$ M 138.123
Needles. Mp 229-230° (227°).
Toda, T., *Bull. Chem. Soc. Jpn.*, 1967, **40**, 588 (*synth, ir, uv*)

2,5-Dihydroxy-2,4,6-cycloheptatrien-1-one, 9CI D-80309

2,5-Dihydroxytropone. 5-Hydroxytropolone
[15852-34-3]
$C_7H_6O_3$ M 138.123
Cryst. by subl. Mp 246-247°.
Russell, G.A. *et al*, *J. Org. Chem.*, 1978, **43**, 3278 (*synth, pmr*)

ent-1α,10β-Dihydroxy-9α,15α-cyclo-20-nor-16-gibberellene-7,19-dioic acid 10,19-lactone D-80310

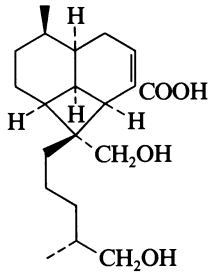


$C_{19}H_{22}O_5$ M 330.380
Antheridiogenin from the fern *Anemia mexicana*. Needles. Mp 213-214°. $[\alpha]_D^{21}$ −72° (c, 0.013 in MeOH).

Furber, M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4084 (*synth*)
Furber, M. *et al*, *Phytochemistry*, 1989, **28**, 63 (*isol*)

1,18-Dihydroxy-14-decipien-19-oic acid D-80311

[76337-44-5]

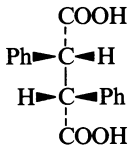


$C_{20}H_{32}O_4$ M 336.470
Isol. from an *Eremophila* sp. Needles (Me_2CO). Mp 133-134°. $[\alpha]_D$ +7° (c, 1.02 in $CHCl_3$).

Croft, K.D. *et al*, *Aust. J. Chem.*, 1980, **33**, 1529 (*isol, pmr, cmr, ms, cryst struct*)

2,3-Dihydroxy-2,3-diphenylbutanedioic acid, 9CI D-80312

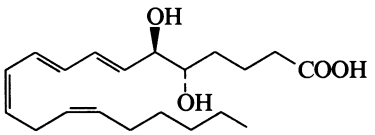
Diphenyltartaric acid



$C_{16}H_{14}O_6$ M 302.283
(2RS,3RS)-form
(±)-threo-*form*
Di-Et ester: [120915-13-1].
$C_{20}H_{22}O_6$ M 358.390
Cryst. (C_6H_6/hexane). Mp 122.5-123°.

Ohgo, Y. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1583 (*synth, cryst struct*)

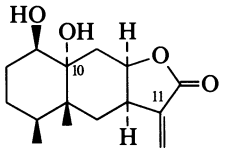
5,6-Dihydroxy-7,9,11,14-eicosatetraenoic acid D-80313



$C_{20}H_{32}O_4$ M 336.470
(5S,6R,7E,9E,11Z,14Z)-form
Metab. of arachidonic acid derived from Leucotriene A_4.
Me ester:
$C_{21}H_{34}O_4$ M 350.497
Oil. $[\alpha]_D^{20}$ +0.91° (c, 0.44 in $CHCl_3$). Other diastereoisomers also prepd.

Nicolaou, K.C. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 587 (*synth, ir, uv, pmr*)

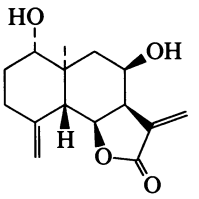
1,10-Dihydroxy-11(13)-eremophilen-12,8-olide D-80314



$C_{15}H_{22}O_4$ M 266.336
(1β,8β,10α)-form
Constit. of *Ondetia linearis*. Oil. $[\alpha]_D^{24}$ +43° (c, 1.14 in $CHCl_3$).
11β,13-Dihydro: 1β,10α-Dihydroxy-11βH-eremophilan-12,8β-olide
$C_{15}H_{24}O_4$ M 268.352
Constit. of *O. linearis*. Gum.
10-Deoxy, 10α-chloro: 10α-Chloro-1β-hydroxy-11(13)-eremophilen-12,8β-olide
$C_{15}H_{21}ClO_3$ M 284.782
Constit. of *O. linearis*. Cryst. Mp 203°. $[\alpha]_D^{24}$ +41° (c, 0.46 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

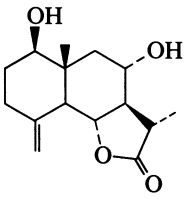
1,8-Dihydroxy-4(15),11(13)-eudesmadien-12,6-olide D-80315



$C_{15}H_{20}O_4$ M 264.321
(1α,5β,6β,8β,10α)-form
Constit. of *Pegolettia oxydonta*. Gum.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1949.

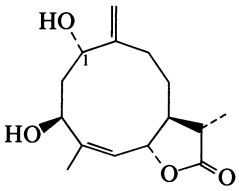
1,8-Dihydroxy-4(15)-eudesmen-12,6-olide D-80316



$C_{15}H_{22}O_4$ M 266.336
(1β,6α,8α,11S)-form
Constit. of *Artemisia gypsacea*.

Fernandez, I. *et al*, *Tetrahedron*, 1987, **43**, 805 (*synth*)
Rustaiyan, A. *et al*, *Phytochemistry*, 1989, **28**, 1535 (*isol*)

1,3-Dihydroxy-4,10(14)-germacradien-12,6-olide D-80317



(1α,3β,4Z,6α,11βH)-*form*

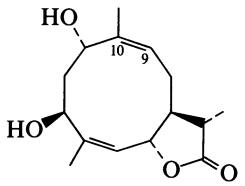
$C_{15}H_{22}O_4$ M 266.336

(1α,3β,4Z,6α,11βH)-form [105304-94-7]
Constit. of *Pyrethrum santalinoides*.

(1β,3β,4Z,6α,11βH)-form [120163-08-8]
Constit. of *P. santalinoides*. Gum. $[\alpha]_D$ +46° (c, 0.18 in $CHCl_3$).

El-Sebakhy, Y. *et al*, *Pharmazie*, 1986, **41**, 525 (*isol*)
Abdel-Mogib, M. *et al*, *Phytochemistry*, 1989, **28**, 268 (*isol*)

1,3-Dihydroxy-4,9-germacradien-12,6-olide D-80318



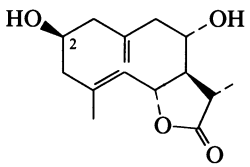
$C_{15}H_{22}O_4$ M 266.336

(1α,3β,4Z,6α,9Z,11βH)-form [120172-53-4]
Constit. of *Pyrethrum santalinoides*. Cryst. Mp 163°. $[\alpha]_D^{24}$ +154° (c, 0.13 in $CHCl_3$).

9β,10β-Epoxide: [120181-04-6]. *9β,10β-Epoxy-1α,3β-dihydroxy-4Z-germacren-12,6α-olide*
$C_{15}H_{22}O_5$ M 282.336
Constit. of *P. santalinoides*. Gum. $[\alpha]_D^{24}$ +34° (c, 0.21 in $CHCl_3$).

Abdel-Mogib, M. *et al*, *Phytochemistry*, 1989, **28**, 268.

2,8-Dihydroxy-4,10(14)-germacradien-12,6-olide D-80319



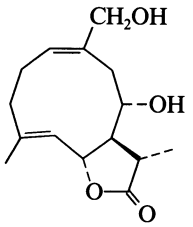
$C_{15}H_{20}O_4$ M 264.321

(2β,6α,8α,11S)-form
11β,13-Dihydroanhydroverlotorin
Constit. of *Artemisia gypsacea*. Gum. $[\alpha]_D^{24}$ +83° (c, 0.45 in $CHCl_3$).

2-Ketone: 8α-Hydroxy-2-oxo-4,10(14)-germacradien-12,6α-olide. ***11β,13-Dihydroartemorin***
$C_{15}H_{18}O_4$ M 262.305
Constit. of *A. gypsacea*. Gum. $[\alpha]_D^{24}$ +48° (c, 0.3 in $CHCl_3$).

Rustaiyan, A. *et al*, *Phytochemistry*, 1989, **28**, 1535.

8,14-Dihydroxy-1(10),4-germacradien-12,6-olide D-80320

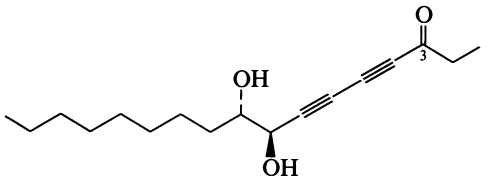


$C_{15}H_{22}O_4$ M 266.336

(1(10)E,4E,6α,8α,11S)-form
8α,14-Dihydroxy-11,13-dihydromelampolide
Constit. of *Artemisia gypsacea*. Gum. $[\alpha]_D^{24}$ +16° (c, 0.2 in $CHCl_3$).

Rustaiyan, A. *et al*, *Phytochemistry*, 1989, **28**, 1535.

8,9-Dihydroxy-4,6-heptadecadiyn-3-one D-80321
Panaxacol



$C_{17}H_{26}O_3$ M 278.391
Isol. from callus of *Panax ginseng*.

3-Alcohol: 4,6-Heptadecadiyne-3,8,9-triol. ***Dihydropanaxacol***
$C_{17}H_{28}O_3$ M 280.406
Isol. from *P. ginseng*.

Fujimoto, Y. *et al*, *Phytochemistry*, 1987, **26**, 2850.

4′,7-Dihydroxyisoflavanone D-80322

Updated Entry replacing D-04539

2,3-Dihydro-7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. Dihydrodaidzein

[17238-05-0]

$C_{15}H_{12}O_4$ M 256.257

(R)-form [58865-02-4]
Constit. of *Pericopsis* spp. Cryst. Mp 201°.

Di-Ac:
$C_{19}H_{16}O_6$ M 340.332
Cryst. (MeOH). Mp 153°. $[\alpha]_D^{24}$ −20.7° ($CHCl_3$).

4′-Me ether: [4626-22-6]. *7-Hydroxy-4′-methoxyisoflavanone. Dihydroformononetin*
$C_{16}H_{14}O_4$ M 270.284
Constit. of *Myroxylon balsamum* trunkwood. Cryst. (EtOH). Mp 185-188°. No opt. rotn. given.

4′-Me ether, 7-O-glucoside: 2,3-Dihydroononin
$C_{22}H_{24}O_9$ M 432.426
Constit. of roots of *Ononis spinosa*. Mp 269-271°.

Di-Me ether: Cryst. (EtOH). Mp 129-130°.

[71815-35-5]

Donnelly, D.M.X. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 186 (*isol, struct, synth*)
Haźnagy, A. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1978, **311**, 318 (*Dihydroononin*)
de Oliveira, A.B. *et al*, *Phytochemistry*, 1978, **17**, 593 (*Dihydroformononetin*)
Jain, A.C. *et al*, *Indian J. Chem., Sect. B*, 1987, **26**, 136 (*synth*)

4′,7-Dihydroxyisoflavone D-80323

Updated Entry replacing D-60340

Daidzein. Dimethylbiochanin B. *Daizeol*

[486-66-8]

$C_{15}H_{10}O_4$ M 254.242

Widespread isoflavone in the Leguminosae (Papilionoideae) eg. in *Chamaecytisus* spp., *Cytisus* spp., *Phaseolus* spp. Also from *Streptomyces xanthophaeus*. Pale-yellow cryst. (EtOH aq.). Mp 330° (323°). Tatoin was impure Daidzein.

Di-Ac: [3682-01-7].
$C_{19}H_{14}O_6$ M 338.316
Cryst. (EtOH). Mp 188-189°.

7-O-β-D-Glucopyranosyl: [552-66-9]. ***Daidzin***
$C_{21}H_{20}O_9$ M 416.384
Isol. from soya bean meal, roots of *P. lobata* and shoots of *Piptanthus nepalensis*. Also from *Baptisia* spp., *Colycine max*, *Medicago sativa*, *Thermopsis* spp. andothers in Leguminosae. Cryst. + $1H_2O$ (H_2O) becoming anhyd. at 120°. Mp 233-235°. $[\alpha]_D^{20}$ −36.4° (0.02N KOH).

4′,7-Di-O-β-D-glucopyranosyl: [53681-67-7].
$C_{27}H_{30}O_{14}$ M 578.526
Stress metab. of cell cultures of *Vigna angularis*. Isol. also from *P. nepalensis*. Needles. Mp 241°.

7-O-(Apiosyl-(1→6)-β-D-glucopyranoside): [108044-04-8]. ***Ambonin***
$C_{26}H_{28}O_{13}$ M 548.499
Constit. of *Neorautanenia amboensis*. Rosettes (Me_2CO aq.). Mp 225-227°. $[\alpha]_D$ −71° (c, 0.014 in H_2O).

4′-Apioside, 7-β-D-glucopyranoside: [108069-01-8]. ***Neobanin***
$C_{26}H_{28}O_{13}$ M 548.499
From *N. amboensis*. Rosettes ($CHCl_3$/MeOH). Mp 211-212°. $[\alpha]_D$ −72.6° (c, 0.018 in H_2O).

4′-Me ether: see *7-Hydroxy-4′-methoxyisoflavone*, *H*-80190

Di-Me ether: [1157-39-7]. *4′,7-Dimethoxyisoflavone. 4′,7-Di-O-methyldaidzein*
$C_{19}H_{14}O_4$ M 306.317
Isol. from *Dalbergia violacea* and *Pterodon apparicioi* heartwoods. Cryst. (EtOH). Mp 162-164° (154-156°).

7-O-(6-O-Acetyl-β-D-glucopyranoside): ***6″-O-Acetyldaidzin***
$C_{23}H_{22}O_{10}$ M 458.421
Isol. from seeds of *G. max*. Needles. Mp 186-189°.

4′-O-β-D-Glucopyranoside:
$C_{21}H_{20}O_9$ M 416.384
Isol. from twigs of *P. nepalensis*.

7-O-Rhamnoside:
$C_{21}H_{20}O_8$ M 400.384
Metab. of *Streptomyces xanthophaeus*. Isolation dubious.

7-O-(Rhamnosylglucoside):
$C_{27}H_{30}O_{13}$ M 562.526
Isol. from leaves and stems of *Baptisia* spp.

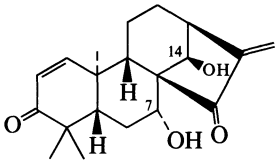
4′,7-Di-O-rhamnoside:
$C_{27}H_{30}O_{12}$ M 546.527
Metab. of *S. xanthophaeus*.

2,3-Dihydro: see *4′,7-Dihydroxyisoflavanone*, *D*-80322

Farkas, L. *et al*, *Chem. Ber.*, 1959, **92**, 819 (*synth*)
Markham, K.R. *et al*, *Phytochemistry*, 1968, **7**, 791 (*isol*)
Gupta, S.R. *et al*, *Phytochemistry*, 1971, **10**, 877 (*synth*)
Dement, W.A., *Phytochemistry*, 1972, **11**, 1089 (*isol*)
Inone, T. *et al*, *Chem. Pharm. Bull.*, 1974, **22**, 1422 (*biosynth*)
Deshpande, V.H. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 201 (*isol*)
Nakayama, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1978, **51**, 2398 (*synth*)
Ohta, N. *et al*, *Agric. Biol. Chem.*, 1979, **43**, 1415 (6″-*O*-Acetyldaidzin)
Jha, H.C. *et al*, *Can. J. Chem.*, 1980, **58**, 1211 (*cmr*)
Ayabe, S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1982, 2725 (*biosynth, ms*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Kobayashi, M. *et al*, *Phytochemistry*, 1983, **22**, 1257 (*isol*)
Jain, A.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1986, 215 (*synth*)
Breytenbach, J.C., *J. Nat. Prod.* (*Lloydia*), 1986, **49**, 1003 (*isol, deriv*)

ent-7β,14α-Dihydroxy-1,16-kauradiene-3,15-dione D-80324

Liangshanin A



$C_{20}H_{26}O_4$ M 330.423

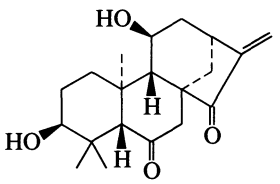
Constit. of *Rabdosia liangshanica*. Needles. Mp 238-240°. $[\alpha]_D$ −192.5° (c, 0.52 in $CHCl_3$).

7-Ac: ent-7β-*Acetoxy*-14α-*hydroxy*-1,16-*kauradiene*-3,15-*dione*. ***Liangshanin C***
$C_{22}H_{28}O_5$ M 372.460
Constit. of *R. liangshanica*. Cryst. Mp 204-210°.

14-Ac: ent-14α-*Acetoxy*-7β-*hydroxy*-1,16-*kauradiene*-3,15-*dione*. ***Liangshanin B***
$C_{22}H_{28}O_5$ M 372.460
Constit. of *R. liangshanica*. Cryst. Mp 204-210°.

Fenglei, Z. *et al*, *Phytochemistry*, 1989, **28**, 1671.

ent-3α,11α-Dihydroxy-16-kaurene-6,15-dione D-80325

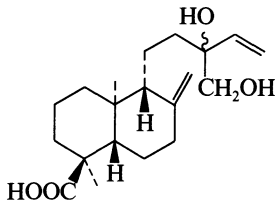


$C_{20}H_{28}O_4$ M 332.439

3-Ac: ent-3α-*Acetoxy*-11α-*hydroxy*-16-*kaurene*-6,15-*dione*. ***Inflexarabdonin C***
$C_{22}H_{30}O_5$ M 374.476
Constit. of *Rabdosia inflexa*. Cryst. (MeOH). Mp 179-181°. $[\alpha]_D^{24}$ −55.2° (c, 0.87 in MeOH).

Takeda, Y. *et al*, *Phytochemistry*, 1989, **28**, 2423 (*isol, pmr, cmr*)

ent-13,16-Dihydroxy-8(17),14-labdadien-18-oic acid D-80326



$C_{20}H_{32}O_4$ M 336.470

Constit. of fruits of *Xylopia aromatica*.

Moraes, M.P.L. *et al*, *Phytochemistry*, 1988, **27**, 3205.

2,13-Dihydroxy-8,14-labdadien-7-one D-80327

$C_{20}H_{32}O_3$ M 320.471

(2α,13R)-form

Constit. of *Waitzia acuminata*.

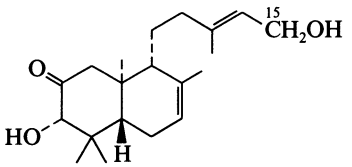
2-Ketone: ***13R-Hydroxy-8,14-labdadiene-2,7-dione***

$C_{20}H_{30}O_3$ M 318.455

Constit. of *W. acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

ent-3β,15-Dihydroxy-7,13-labdadien-2-one D-80328



$C_{20}H_{32}O_3$ M 320.471

Constit. of *Baccharis boliviensis*. Gum.

15-Aldehyde: **ent-*3β-Hydroxy-2-oxo-7,13-labdadien-15-al***

$C_{20}H_{30}O_3$ M 318.455

Constit. of *B. boliviensis*. Oil. Both *E*- and *Z*-isomers occur.

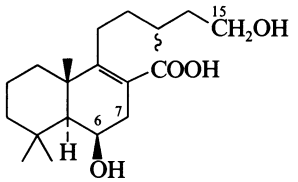
15-Aldehyde, 3-deoxy: **ent-*2-Oxo-7,13-labdadien-15-al***

$C_{20}H_{30}O_2$ M 302.456

Constit. of *B. boliviensis*. Oil.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

6,15-Dihydroxy-8-labden-17-oic acid D-80329



$C_{20}H_{34}O_4$ M 338.486

6β-form

Constit. of *Halimium verticillatum*.

Urones, J.G. *et al*, *Phytochemistry*, 1989, **28**, 557.

7,15-Dihydroxy-8-labden-17-oic acid D-80330

$C_{20}H_{34}O_4$ M 338.486

7α-form

7-Me ether: 15-Hydroxy-7α-methoxy-8-labden-17-oic acid

$C_{21}H_{36}O_4$ M 352.513

Constit. of *Halimium verticillatum*.

7-Me ether, 15-Ac, Me ester: Oil. $[\alpha]_D^{22}$ +21.36° (c, 1.1 in $CHCl_3$).

7β-form

Di-Ac: 7β,15-Diacetoxy-8-labden-17-oic acid

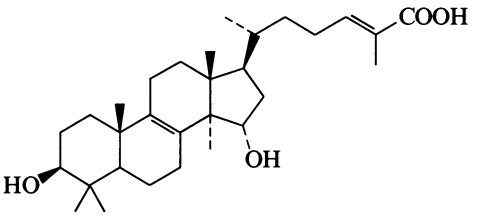
$C_{24}H_{38}O_6$ M 422.561

Constit. of *H. verticillatum*.

Di-Ac, Me ester: Oil. $[\alpha]_D^{22}$ +24.0° (c, 1.32 in $CHCl_3$).

Urones, J.G. *et al*, *Phytochemistry*, 1989, **28**, 557.

3,15-Dihydroxy-8,24-lanostadien-26-oic acid D-80331



$C_{30}H_{48}O_4$ M 472.707

(3β,15α,24E)-form

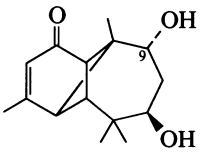
Di-Ac: [117842-20-3]. *3β,15α-Diacetoxy-8,24-lanostadien-26-oic acid*

$C_{34}H_{52}O_6$ M 556.781

Constit. of *Ganoderma lucidum*.

Lin, L.-J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 919.

7,9-Dihydroxy-2-longipinen-1-one D-80332



(7β,9α)-*form*

$C_{15}H_{22}O_3$ M 250.337

(7β,9α)-form [97335-21-2]

Constit. of *Lavandula stoechas* and *Stevia salicifolia*. Cryst. ($CHCl_3$). Mp 183-184°. $[\alpha]_D$ +48° (c, 2 in EtOH).

9-Ac: 9α-Acetoxy-7β-hydroxy-2-longipinen-1-one

$C_{17}H_{24}O_4$ M 292.374

Constit. of *L. stoechas*.

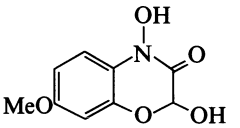
Roman, L.U. *et al*, *J. Org. Chem.*, 1985, **50**, 3965 (*isol, struct*)
Ulubelen, A. *et al*, *Phytochemistry*, 1988, **27**, 3966 (*isol, deriv*)

2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one D-80333

Updated Entry replacing D-10388

DIMBOA

[15893-52-4]



$C_9H_9NO_5$ M 211.174

Isol. from wheat, in which it is present mainly as glucoside. Appears to be a natural aphicide and fungicide. Involved in the *in vivo* detoxification of herbicides, e.g. Simazine. Pink needles. Mp 156-157° dec.

O-β-D-Glucoside:

$C_{15}H_{19}NO_{10}$ M 373.316

Isol. from wheat (*Zea mays*). Needles (EtOH). Mp 262-263° dec.

Demethoxy: 2,4-Dihydroxy-2H-1,4-benzoxazin-3(4H)-one

$C_8H_7NO_4$ M 181.148

Isol. from rye (*Secale cereale*) and maize (*Z. mays*). Cryst. (Et_2O/cyclohexane). Mp 152°.

Demethoxy, 2-O-β-D-glucoside:

$C_{14}H_{17}NO_9$ M 343.290

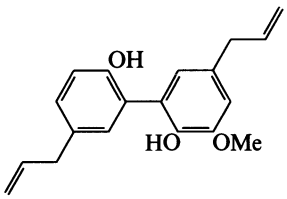
Isol. from *S. cereale* and *Z. mays*. Cryst. Mp 186.5-187°.

Wahlroos, O. *et al*, *Acta Chem. Scand.*, 1959, **13**, 1906 (*isol, struct*)

Virtanen, A.L. *et al*, *Acta Chem. Scand.*, 1960, **14**, 499, 502, 504 (*isol, synth, derivs*)
Reimann, J.E. *et al*, *Biochemistry*, 1964, **3**, 847 (*biosynth*)
Hofman, J. *et al*, *Tetrahedron Lett.*, 1969, 5001 (*isol, uv, glucoside*)
Argandoã, V.H. *et al*, *Phytochemistry*, 1980, **19**, 1665; 1981, **20**, 673 (*isol*)

2,2′-Dihydroxy-3-methoxy-5,5′-di-2-propenylbiphenyl D-80334

5,5′-Diallyl-2,2′-dihydroxy-3-methoxybiphenyl

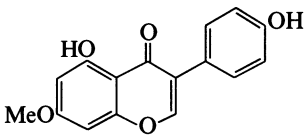


$C_{19}H_{20}O_3$ M 296.365
Constit. of *Magnolia henryi*. Gum.

Kijjoa, A. *et al*, *Phytochemistry*, 1989, **28**, 1284.

4′,5-Dihydroxy-7-methoxyisoflavone D-80335

Updated Entry replacing D-10392
Prunetin. *Padmakastein. Prunusetin*
[26015-63-4]



$C_{16}H_{12}O_5$ M 284.268
Occurs in bark of *Prunus puddum* and in several other *P.* spp. (Rosaceae) and in *Genista violacea, G. carinalis, Glycyrrhiza glabra* and *Pterocarpus angolensis* (Leguminosae). Also prod. by cultures of *Mycobacterium phlei*. Cryst. (EtOH). Mp 236-238°. All isolations of isoflavones from microorganism cultures are considered doubtful.

4′-O-β-D-Glucopyranoside: [154-36-9]. ***Prunitrin.*** *Prunitroside. Trifoside. Prunetrin*
$C_{22}H_{22}O_{10}$ M 446.410
Isol. from *P. mahaleb, P. puddum, Trifolium medium, T. pratense* and *Genista carinalis*. Reported to have antispasmodic, expectorant and hypolipidaemic props. Mp 181° (sinters from 160°). $[\alpha]_D$ −82.5° (Py). Padmakastin was prob. impure prunitrin.

Hasegawa, M., *J. Am. Chem. Soc.*, 1957, **79**, 1738 (*isol*)
Plouvier, V. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1960, **250**, 594 (*isol, deriv*)
Hudson, A.T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 830 (*isol*)
Farkas, L. *et al*, *Tetrahedron*, 1969, **25**, 1013 (*struct, synth*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

4′,7-Dihydroxy-5-methoxyisoflavone D-80336

7-Hydroxy-3-(4-hydroxyphenyl)-5-methoxy-4H-1-benzopyran-4-one, 9CI. ***Isoprunetin.*** *5-O-Methylgenistein*
[4569-98-6]
$C_{16}H_{12}O_5$ M 284.268
Isol. from a wide variety of spp. in Leguminosae subf. Papilionoideae, eg. *Adenocarpus, Chamaecytisus, Cytisus, Genista* and *Ulex* spp. Needles. Mp 302° (290°) dec.

Chopin, J. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 1038 (*isol, ir, uv, struct, synth*)
Harborne, J.B., *Phytochemistry*, 1969, **8**, 1449 (*occur*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*occur*)

5,7-Dihydroxy-4′-methoxyisoflavone D-80337

Updated Entry replacing D-04603
5,7-Dihydroxy-3-(4-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Biochanin A.*** *Genistein 4′-methyl ether. Pratensol*
[491-80-5]
$C_{16}H_{12}O_5$ M 284.268
Constit. of clover (*Trifolium repens*), *Dalbergia* and *Cotoneaster* spp. Widely distributed in the Leguminosae (Papilionoideae), also in *Cotoneaster pannosa* and *C. serotina* (Rosaceae) and *Virola caducifolia* (Myricaceae). Sl. oestrogenic. Needles (MeOH or EtOH aq.). Mp 215-216°.

7-Ac: Rectangular plates (MeOH). Mp 155-156°.

5,7-Di-Ac: Needles (MeOH). Mp 190°.

7-β-D-Glucoside: [5928-26-7]. ***Sissotrin.*** *Astroside*
$C_{22}H_{22}O_{10}$ M 446.410
Constit. of *Thermopsis* and *C.* spp., also from *Astragalus austriacus, Baptisia leucantha, Cicer arietinum, Pueraria thumbergiana, Sophora japonica* and *Trifolium*spp. Mp 220°. $[\alpha]_D^{30}$ −35.3° (c, 1.644 in DMF).

7-(β-D-Apiosyl(1→2)-β-D-glucopyranoside): [15914-68-8]. ***Lanceolarin***
$C_{27}H_{30}O_{14}$ M 578.526
Constit. of the root bark of *D. lanceolaria*. Cryst. (MeOH). Mp 165-167° (unsharp, previous sintering). $[\alpha]_D^{22}$ −96.9° (c, 1.032 in 80% MeOH aq.).

7-O-Rhamnosylglucoside:
$C_{28}H_{32}O_{14}$ M 592.552
Isol. from *B.* spp.

7-O-Rutinoside:
$C_{28}H_{32}O_{14}$ M 592.552
Isol. from *D. paniculata* bark. Thin rods + $3H_2O$ (MeOH). Mp 153-154°. $[\alpha]_D^{20}$ −51.9° (c, 1 in MeOH).

7-O-Gentiobioside:
$C_{28}H_{32}O_{15}$ M 608.552
Isol. from wood of *S. japonica*. Prisms (MeOH aq.). Mp 224-226°. $[\alpha]_D^{24}$ −38.7° (c, 1.79 in 80% MeOH aq.).

7-O-(Xylosylglucoside): Isol. from *S. japonica* wood. Needles (MeOH aq.). Mp 228-230°. $[\alpha]_D^{24}$ −79.5° (c, 0.52 in 80% MeOH aq.).

7-O-(6-O-Malonyl-D-glucoside):
$C_{25}H_{24}O_{13}$ M 532.457
Isol. from leaves of *Trifolium pratense* and *T. subterranium*. Needles (MeOH). Mp 217°. Revised struct.

7-O-(6-O-Malonyl-D-glucoside), Me ester:
$C_{26}H_{26}O_{13}$ M 546.484
Isol. from leaves of *T. pratense* and *T. subterraneum*. Needles (MeOH). Mp 195°.

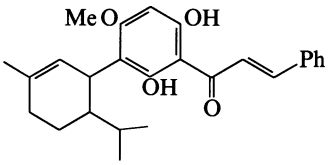
Baker, W. *et al*, *J. Chem. Soc.*, 1953, 1852 (*synth*)
Geissman, T.A. *et al*, *Phytochemistry*, 1965, **4**, 89 (*Sissotrin*)
Malhotra, A. *et al*, *Tetrahedron*, 1967, **23**, 405 (*Lanceolarin*)
Beck, A.B. *et al*, *Aust. J. Chem.*, 1971, **24**, 1509 (*malonates*)
Parthasarathy, M.R. *et al*, *Phytochemistry*, 1976, **15**, 1025 (*rutinoside*)
Foot, S. *et al*, *Synthesis*, 1976, 326 (*synth*)
Diedrich, D.F. *et al*, *J. Chem. Eng. Data*, 1977, **22**, 448 (*pmr*)
Takeda, T. *et al*, *Phytochemistry*, 1977, **16**, 619 (*xylosylglucoside, gentiobioside*)

Bass, R.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1978, 666 (*cmr*)
Ashdown, D.H.J. *et al*, *Synthesis*, 1978, 843 (*synth*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

2′,6′-Dihydroxy-4′-methoxy-3′-(1-p-menthen-3-yl)chalcone D-80338

1-[2,6-Dihydroxy-4-methoxy-3-[3-methyl-6-(1-methylethyl)-2-cyclohexen-1-yl]phenyl]-3-phenyl-2-propen-1-one, 9CI. 2′,6′-Dihydroxy-4′-methoxy-3′-(3-methyl-6-methylethyl-2-cyclohexenyl)chalcone

[119628-53-4]



$C_{26}H_{30}O_4$ M 406.521
Constit. of *Lindera umbellata*. Yellow powder. $[\alpha]_D^{20}$ +119.7° (c, 0.76 in $CHCl_3$).

Shimomura, H. *et al*, *Phytochemistry*, 1988, **27**, 3937.

4,5-Dihydroxy-2-methylbenzoic acid D-80339

$C_8H_8O_4$ M 168.149

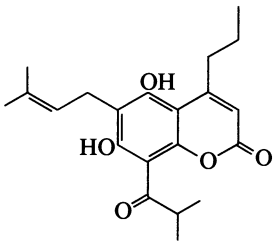
Di-Me ether: [20736-28-1]. *4,5-Dimethoxy-2-methylbenzoic acid*
$C_{10}H_{12}O_4$ M 196.202
Cryst. (EtOH aq.). Mp 139-141°.

Di-Me ether, N,N-*diethylamide:* [113975-92-1].
$C_{14}H_{21}NO_3$ M 251.325
Oil.

Clark, R.D. *et al*, *J. Org. Chem.*, 1988, **53**, 2378 (*derivs, synth, pmr*)

5,7-Dihydroxy-7-(3-methyl-2-butenyl)-8-(2-methyl-2-oxopropyl)-3-propyl-2*H*-1-benzopyran-2-one D-80340

5,7-Dihydroxy-8-(2-methyl-1-oxopropyl)-7-prenyl-3-propylcoumarin



$C_{21}H_{26}O_5$ M 358.433
Isol. from *Mammea americana*. Related to the Mammeins.

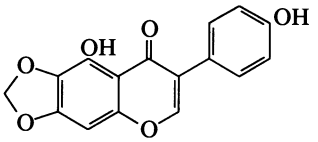
Games, D.E. *et al*, *Tetrahedron Lett.*, 1972, 3187.

4′,5-Dihydroxy-6,7-methylenedioxyisoflavone D-80341

Updated Entry replacing D-04712

*9-Hydroxy-7-(4-hydroxyphenyl)-8*H*-1,3-dioxolo[4,5-g][1]benzopyran-8-one, 9CI.* ***Irilone***

[41653-81-0]



$C_{16}H_{10}O_6$ M 298.251
Constit. of *Iris germanica* and of *Trifolium pratense*. Yellow cryst. Mp 231°.

4′-O-Glucoside: [50868-47-8]. *Irilone-4′-glucoside*
$C_{22}H_{20}O_{11}$ M 460.393
Isol. from rhizomes of *Iris florentina* and roots of *Trifolium pratense*. Needles ($CHCl_3$/MeOH)(as pentaacetate). Mp 233-235° (pentaacetate).

5-Me ether: [3301-68-6]. *4′-Hydroxy-5-methoxy-6,7-methylenedioxyisoflavone.* ***Irisolone***
$C_{17}H_{12}O_6$ M 312.278
Isol. from *I. florentina*, *I. germanica* and *I. nepalensis*. Plates (EtOAc/2-methoxyethanol). Mp 269-270°.

5-Me ether, 4′-O-glucosylglucoside: [50938-05-1]. *Irisolone-4′-bioside*
$C_{29}H_{32}O_{16}$ M 636.562
Isol. from rhizomes of *I. florentina*. Cryst (MeOH)(as heptaacetate). Mp 173-175° (heptaacetate).

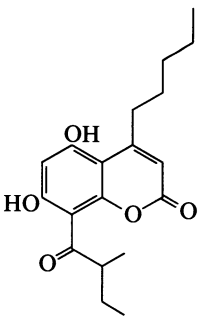
Di-Me ether: [3405-76-3]. *4′,5-Dimethoxy-6,7-methylenedioxyisoflavone. Irisolone methyl ether*
$C_{18}H_{14}O_6$ M 326.305
Isol. from bulbs of *I. tingitana*. Mp 180-183°.

Gopinath, K.W. *et al*, *Tetrahedron*, 1961, **16**, 201 (*isol, struct*)
Arisawa, M. *et al*, *Chem. Pharm. Bull.*, 1973, **21**, 2323 (*isol, deriv*)
Pailer, M. *et al*, *Monatsh. Chem.*, 1973, **104**, 1394 (*isol, deriv*)
Tsukida, K. *et al*, *Phytochemistry*, 1973, **12**, 2318 (*glycosides*)
Dhar, K.L. *et al*, *Phytochemistry*, 1973, **12**, 734 (*isol, uv*)
El-Emary, N.A. *et al*, *Phytochemistry*, 1980, **19**, 1878 (*isol, deriv*)

5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-4-one, 9CI D-80342

5,7-Dihydroxy-8-(2-methylbutyryl)-4-pentylcoumarin

[36478-56-5]

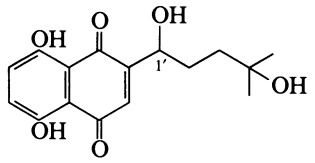


$C_{19}H_{24}O_5$ M 332.396
Isol. from *Mammea africana*. Mp 218-220°. Related to the Mammeins.

Carpenter, I. *et al*, *J. Chem. Soc. C*, 1971, 3783.

2-(1,4-Dihydroxy-4-methylpentyl)-5,8-dihydroxy-1,4-naphthoquinone D-80343

Updated Entry replacing A-00173



$C_{16}H_{18}O_6$ M 306.315

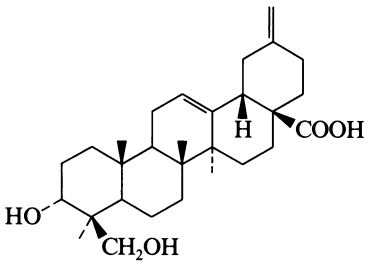
1'-Ac: [34232-25-2]. ***Arnebin VI.*** *2-(1-Acetoxy-4-hydroxy-4-methylpentyl)-5,8-dihydroxy-1,4-naphthoquinone*
$C_{18}H_{20}O_7$ M 348.352
Constit. of *Arnebia nobilis*. Mp 88-90°.

1'-(4-Methyl-2-butenoyl): [36883-11-1]. ***Arnebin II***
$C_{21}H_{24}O_7$ M 388.416
Major quinone from roots of *A. nobilis*. Dark red needles. Mp 92-94°.

1'-Deoxy: ***Arnebin V.*** *5,8-Dihydroxy-2-(4-hydroxy-4-methylpentyl)naphthoquinone*
$C_{16}H_{18}O_5$ M 290.315
Isol. from *A. nobilis*. Mp 111-112°.

Shukla, Y.N. *et al*, *Phytochemistry*, 1971, **10**, 1909 (*isol, struct*)

3,24-Dihydroxy-30-nor-12,20(29)-oleanadien-28-oic acid D-80344



$C_{29}H_{44}O_4$ M 456.664

3α-form [119863-89-7] ***Quinatic acid***
Constit. of *Akebia quinata* callus tissue. Needles. Mp 269-272°. $[\alpha]_D^{18}$ +66.6° (c, 0.375 in Py).

Ikuta, A. *et al*, *Phytochemistry*, 1988, **27**, 3809.

4,14-Dihydroxyoctadecanoic acid D-80345

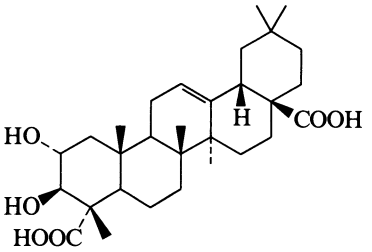
$H_3C(CH_2)_3CH(OH)(CH_2)_9CH(OH)CH_2CH_2COOH$

$C_{18}H_{34}O_4$ M 314.464

14-O-Diglucoside, Et ester: ***Muricatin A***
$C_{32}H_{21}O_{10}$ M 565.512
Isol. from *Ipomoeia muricata*. Mp 117-118°. $[\alpha]_D^{28}$ −29.8° (EtOH). Complete struct. not known. Muricatin A is not homogeneous.

Khanna, S.N. *et al*, *Phytochemistry*, 1967, **6**, 735.

2,3-Dihydroxy-12-oleanene-23,28-dioic acid D-80346



$C_{30}H_{46}O_6$ M 502.690

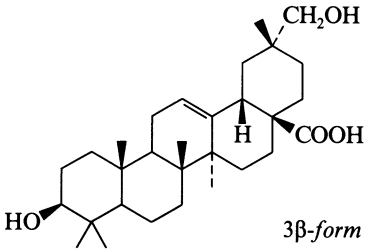
(2α,3β)-form [471-58-9] ***Barringtogenic acid***
Isol. from *Barringtonia* spp. Prisms (MeOH). Mp 332-334° dec. $[\alpha]_D$ +72° (MeOH).

Di-Me ester: Mp 253-254°. $[\alpha]_D^{30}$ +61°.

Anantaraman, R. *et al*, *J. Chem. Soc.*, 1956, 4369.
Sastry, C.S.P. *et al*, *Tetrahedron*, 1967, **23**, 3837.

3,29-Dihydroxy-12-oleanen-28-oic acid D-80347

Updated Entry replacing D-04896



3β-*form*

$C_{30}H_{48}O_4$ M 472.707

3α-form
3-Epimesembryanthemoidigenic acid
Constit. of *S. hexaphylla*.

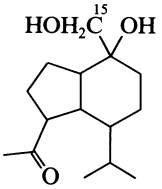
Ac:
$C_{32}H_{50}O_5$ M 514.744
Constit. of *S. hexaphylla*. Amorph. $[\alpha]_D^{18}$ +106.7° (c, 0.03 in $CHCl_3$).

3β-form [4871-87-8] ***Mesembryanthemoidigenic acid***
Constit. of *Rhipsalis mesembryanthemoides*. Cryst. (MeOH). Mp 305-309°. $[\alpha]_D$ +70.7°.

3-Ac: Constit. of *Stauntonia hexaphylla*.

Tursch, B. *et al*, *Tetrahedron Lett.*, 1965, 4161 (*isol, struct*)
Ikuta, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 623 (*isol, pmr, cmr*)

10,15-Dihydroxy-4-oplopanone D-80348

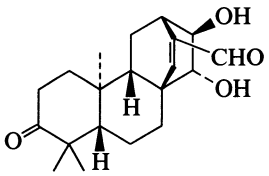


$C_{15}H_{36}O_3$ M 264.448

15-Angeloyl: 15-Angeloyloxy-10-hydroxy-4-oplopanone
$C_{20}H_{32}O_4$ M 336.470
Constit. of *Senecio mexicanus*. Oil. $[\alpha]_D$ −22° (c, 0.17 in $CHCl_3$).

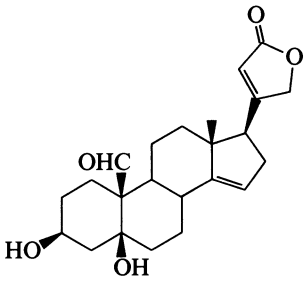
Joseph-Nathan, P. *et al*, *Phytochemistry*, 1989, **28**, 2397 (*isol, pmr, ms*)

ent-13*R*-14*R*-Dihydroxy-3-oxo-15-atisen-17-al D-80349



$C_{20}H_{28}O_4$ M 332.439
Constit. of *Euphorbia fidjiana*. Oil.
Lal, A.R. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3205.

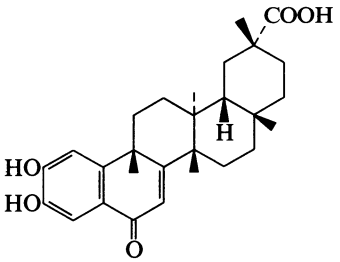
3,5-Dihydroxy-19-oxo-14,20(22)-cardadienolide, 9CI D-80350



$C_{23}H_{30}O_5$ M 386.487
(*3β,5β*)-*form* [806-02-0] ***Diffugenin.*** 14-*Anhydrostrophanthidin*
Aglycone isol. from seeds of *Erysimum diffusum* after hydrol. Needles (EtOH/Et_2O). Mp 186-188°. $[\alpha]_D^{20}$ +5.4° (c, 1.24 in MeOH).
Makarichev, G.K. *et al*, *Zh. Obshch. Khim.*, 1962, **32**, 2372 (*isol, struct*)
Rashkes, Ya.V. *et al*, *Khim. Prir. Soedin.*, 1971, **7**, 747; *Chem. Nat. Compd.*, 724 (*ms*)

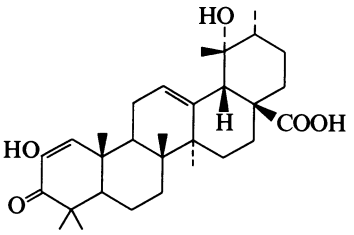
2,3-Dihydroxy-6-oxo-23,24-dinor-1,3,5(10),7-friedelatetraen-29-oic acid D-80351

23-Nor-6-oxodemethylpristimerol
[118172-80-8]



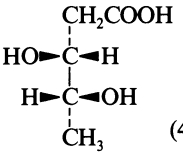
$C_{28}H_{36}O_5$ M 452.589
Constit. of *Kokoona zeylanica*. Yellow solid. Mp 228-230°. $[\alpha]_D^{27}$ −102° ($CHCl_3$).
Me ester: [118172-79-5]. ***23-Nor-6-oxopristimerol***
$C_{29}H_{38}O_5$ M 466.616
Constit. of *K. zeylanica*. Pale yellow solid. Mp 135-138°. $[\alpha]_D^{27}$ −74.9° ($CHCl_3$).
Gamlath, C.B. *et al*, *Phytochemistry*, 1988, **27**, 3221.

2,19-Dihydroxy-3-oxo-1,12-ursadien-28-oic acid D-80352



$C_{30}H_{44}O_5$ M 484.675
19α-form
Fupenzic acid
Constit. of *Rubus chingii*. Needles. Mp 189-190°. $[\alpha]_D^{25}$ +45.6° (c, 0.16 in MeOH).
Hattori, M. *et al*, *Phytochemistry*, 1988, **27**, 3975.

3,4-Dihydroxypentanoic acid D-80353

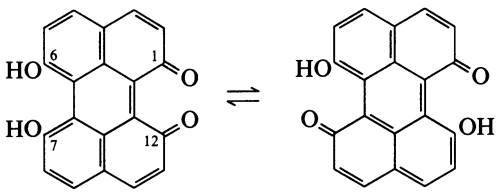


(*4R,5R*)-*form*

$C_5H_{10}O_4$ M 134.132
(***4R,5R***)-***form***
D-threo-form
1,4-Lactone: [38996-24-6]. *Dihydro-4-hydroxy-5-methyl-2(3H)furanone. 2,5-Dideoxy-γ-pentonolactone*
$C_5H_8O_3$ M 116.116
Oil. $[\alpha]_D$ +75° (c, 0.25 in EtOH).
(***4R,5S***)-***form***
L-erythro-form
1,4-Lactone: [98512-76-6].
Liq. Bp_{12} 125°. $[\alpha]_D^{20}$ −10.81° (c, 1.85 in $CHCl_3$).
(***4S,5S***)-***form***
L-threo-form
1,4-Lactone: [105881-47-8].
Oil. $[\alpha]_D^{20}$ −73.7° (c, 1.6 in EtOH).
(***4S,5R***)-***form***
D-erythro-form
1,4-Lactone: [88400-20-8].
Liq. $Bp_{0.025}$ 108-110°. $[\alpha]_D$ +10.87° (c, 2.42 in $CHCl_3$).
Chen, S. *et al*, *J. Org. Chem.*, 1984, **49**, 2168 (*synth, pmr, cmr, ir, ms*)
Moore, R.E. *et al*, *J. Org. Chem.*, 1984, **49**, 2484 (*synth, pmr, cd*)
Ortuño, R.M. *et al*, *Tetrahedron*, 1987, **43**, 2191 (*synth, pmr, ir, ms*)

6,7-Dihydroxy-1,12-perylenedione, 9CI D-80354

[117156-88-4]



$C_{20}H_{10}O_4$ M 314.297
Tautomeric.
6,7-Dihydroxy-form
Di-Ac: [117156-93-1].

$C_{24}H_{14}O_6$ M 398.371
Plates (CH_2Cl_2/MeOH). Mp 218-219° dec.

Di-Me ether: [117156-90-8]. *6,7-Dimethoxy-1,12-perylenedione*
$C_{22}H_{14}O_4$ M 342.350
Dark red needles (CH_2Cl_2/MeOH). Mp 277-279°.

6,12-Dihydroxy-form
6,12-*Dihydroxy*-1,7-*perylenedione*

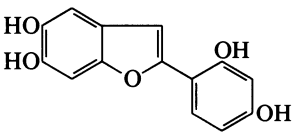
Di-Ac: [117156-92-0].
Red plates (CH_2Cl_2/MeOH). Mp >280° dec.

Di-Me ether: [117156-91-9]. *6,12-Dimethoxy-1,7-perylenedione*
$C_{22}H_{14}O_4$ M 342.350
Dark red microcryst. (CH_2Cl_2/pet. ether). Mp 285-290° dec.

[117156-89-5]

Calderon, J.S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 583 (*synth, ir, uv, pmr, ms*)

2-(2,4-Dihydroxyphenyl)-5,6-dihydroxybenzofuran D-80355



$C_{14}H_{10}O_5$ M 258.230

5,6-Di-Me ether: [67492-33-5]. *2-(2,4-Dihydroxyphenyl)-5,6-dimethoxybenzofuran*
$C_{16}H_{14}O_5$ M 286.284
Isol. from trunkwood of *Myroxylon balsamum*. Mp 178-180°.

5,6-Methylene ether: [67121-26-0]. *2-(2,4-Dihydroxyphenyl)-5,6-methylenedioxybenzofuran*
$C_{15}H_{10}O_5$ M 270.241
Isol. from aerial parts of *Sophora tomentosa*. Plates. Mp 235-237°.

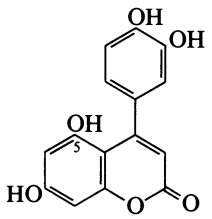
4'-Me, 5,6-methylene ether: 2-(2-Hydroxy-4-methoxyphenyl)-5,6-methylenedioxybenzofuran
$C_{16}H_{12}O_5$ M 284.268
Isol. from aerial parts of *S. tomentosa*. Needles (MeOH). Mp 179-181°.

[67236-31-1]

Komatsu, M. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 1274 (*isol, uv, pmr, struct*)
Braga de Oliviera, A. *et al*, *Phytochemistry*, 1978, **17**, 593 (*isol, ir, uv, pmr, ms, struct*)

4-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2*H*-1-benzopyran-2-one D-80356

4-(3,4-Dihydroxyphenyl)-5,7-dihydroxycoumarin. 3',4',5,7-Tetrahydroxyneoflavone



$C_{15}H_{10}O_6$ M 286.240

5-Me ether: 4-(3,4-Dihydroxyphenyl)-7-hydroxy-5-methoxycoumarin. 3',4',7-Trihydroxy-5-methoxyneoflavone
$C_{16}H_{12}O_6$ M 300.267
Constit. of *Coutarea hexandra*. Cryst. (MeOH). Mp 269-270°.

4',7-Di-Me ether: 5-Hydroxy-4-(3-hydroxy-4-methoxyphenyl)-7-methoxycoumarin. 3',5-Dihydroxy-4',7-dimethoxyneoflavone
$C_{17}H_{14}O_6$ M 314.294
Constit. of *Exostema caribaeum*. Cryst. Mp 225-226°.

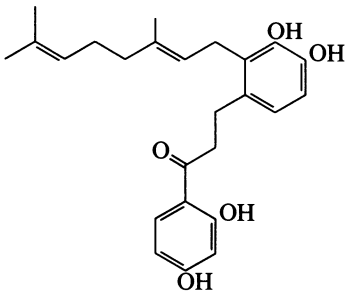
7-Me ether, 5-O-β-D-glucopyranosyl: [116310-58-8]. *5-O-β-D-Glucopyranosyl-3',4'-dihydroxy-7-methoxyneoflavone*
$C_{22}H_{22}O_{11}$ M 462.409
Constit. of *E. caribaeum*. Cryst. (MeOH). Mp 237-238°.

7-Me ether, 5-O-(6-acetyl-β-D-galactopyranosyl): 5-O-(6-Acetyl-β-D-galactopyranosyl)-3',4'-dihydroxy-7-methoxyneoflavone
$C_{24}H_{24}O_{11}$ M 488.447
Constit. of *E. caribaeum*. Cryst. Mp 215-220°.

Mata, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 851 (*isol*)
Delle Monache, G. *et al*, *Heterocycles*, 1989, **29**, 355 (*isol*)

1-(2,4-Dihydroxyphenyl)-3-[3,4-dihydroxy-2-(3,7-dimethyl-2,6-octadienyl)phenyl]-1-propanone D-80357

AC-5-1

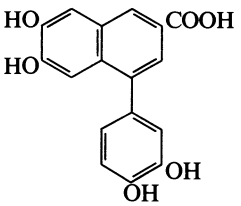


$C_{25}H_{30}O_5$ M 410.509
Constit. of *Artocarpus communis*. 5-Lipoxygenase inhibitor. Powder. Mp 132-136°.

Nakano, J. *et al*, *Heterocycles*, 1989, **29**, 427.

4-(3,4-Dihydroxyphenyl)-6,7-dihydroxy-2-naphthalenecarboxylic acid, 9CI D-80358

[121242-02-2]

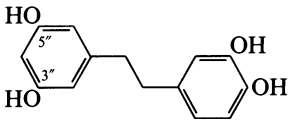


$C_{17}H_{12}O_6$ M 312.278
Constit. of *Pellia epiphylla*. Cryst. (MeOH). Mp 325-327° dec.

Rischmann, M. *et al*, *Phytochemistry*, 1989, **28**, 867.

1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethane D-80359

4-[2-(3,5-Dihydroxyphenyl)ethyl]-1,2-benzenediol

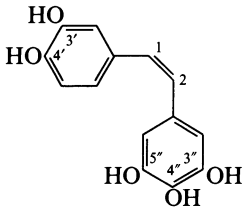


$C_{14}H_{14}O_4$ M 246.262

3″,5″-Di-Me ether: [116518-75-3]. *1-(3,4-Dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)ethane.* ***Combretastatin B4***
$C_{16}H_{18}O_4$ M 274.316
Constit. of *Combretum caffrum*. Viscous oil.

Pettit, G.R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 517.

1-(3,4-Dihydroxyphenyl)-2-(3,4,5-dihydroxyphenyl)ethylene D-80360



$C_{14}H_{12}O_5$ M 260.246

(Z)-form

3′,4′-Di-Me, 4″,5″-methylene ether: [111394-44-6]. ***Combretastatin A2***
$C_{17}H_{16}O_5$ M 300.310
Constit. of *Combretum caffrum*. Oil.

3″,4′,4″-Tri-Me ether: [111394-45-7]. ***Combretastatin A3***
$C_{17}H_{18}O_5$ M 302.326
Constit. of *C. caffrum*. Oil.

3′,4′,4″-Tri-Me ether, 1,2-dihydro: [111394-46-8]. *3,5-Dihydroxy-3′,4,4′-trimethoxybibenzyl.* ***Combretastatin B2***
$C_{17}H_{20}O_5$ M 304.342
Constit. of *C. caffrum*. Oil.

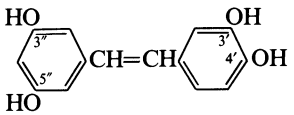
3′,3″,5″-Tri-Me ether, 1,2-dihydro: [108853-14-1]. *4,4′-Dihydroxy-3,3′,5-trimethoxybibenzyl*
$C_{17}H_{20}O_5$ M 304.342
Constit. of *Dendrobium chrysanthum*. Cryst. (Et_2O). Mp 87-89°.

Pettit, G.R. *et al*, *Can. J. Chem.*, 1987, **65**, 2390.
Min, Z.-D. *et al*, *J. Nat. Prod.* (*Lloydia*), 1987, **50**, 1189.

1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene D-80361

Updated Entry replacing D-10420

4-[2-(3,5-Dihydroxyphenyl)ethenyl]-1,2-benzenediol, 9CI.
3,3′,4,5′-Stilbenetetrol, 8CI. 3,3′,4,5′-Tetrahydroxystilbene. ***Piceatannol.*** *Astringenin*



$C_{14}H_{12}O_4$ M 244.246

(E)-form [10083-24-6]

Found in Norway spruce, *Vouacapoua macropetala*, *Pericopsis angolensis* and other spp. Fungal inhibitor. Plant growth inhibitor and ichthyotoxin. Needles (EtOAc/hexane). Mp 231-232° (216°).

Tetra-Ac: Needles (MeOH). Mp 115°, Mp 124° (double Mp).

Tetrabenzoyl: Mp 153-154°.

Tetra-Me ether: Needles (MeOH aq.). Mp 67-69°.

3′-Glucoside: [29884-49-9]. ***Astringin***
$C_{20}H_{22}O_9$ M 406.388
Constit. of *Picea* spp. Also from *Eucalyptus dundasii*.

3′-Me ether: [32507-66-7]. *5-[2-(3-Hydroxy-4-methoxyphenyl)ethenyl]-1,3-benzenediol, 9CI. 3′-Methoxy-3,4′5-stilbenetriol, 8CI. Isorhapontigenin*
$C_{15}H_{14}O_4$ M 258.273
Cryst. (EtOAc/pet. ether). Mp 182-183°.

3′-Me ether, 3″-glucoside: [32727-29-0]. ***Isorhapontin***
$C_{21}H_{24}O_9$ M 420.415
Constit. of *Picea glauca*, *P. koraensis*, *P. obovata* and *P. glehnii*. White-yellow amorph. powder ($MeOH/CHCl_3$). Mp 193-194°. $[\alpha]_D^{21}$ −54.1° (c, 2.24 in Me_2CO).

4′-Me ether: [500-65-2]. *1-(3,5-Dihydroxyphenyl)-2-(3-hydroxy-4-methoxyphenyl)ethylene. 3,3′,5-Trihydroxy-4′-methoxystilbene.* ***Rhapontigenin.*** *Pontigenin*
$C_{15}H_{14}O_4$ M 258.273
Isol. from rhizomes of *Rheum undulatum*. Mp 186-187°.

4′-Me ether, 3′-glucoside: [155-58-8]. ***Rhapontin.*** *Rhaponticin. Ponticin*
$C_{21}H_{24}O_9$ M 420.415
Isol. from seeds of *R. rhaponticum*, *R. emodi* and *Euclalyptus sideroxylon*. Mp 236-237° dec. $[\alpha]_D^{32}$ −59.5° (Me_2CO).

1,2-Dihydro, 3′,3″-di-Me ether: [67884-30-4]. *1-(3-Hydroxy-5-methoxyphenyl)-2-(4-hydroxy-3-methoxyphenyl)ethane.* ***Gigantol***
$C_{16}H_{18}O_4$ M 274.316
Constit. of *Cymbidium giganteum*. Cryst. ($CHCl_3$/pet. ether). Mp 94-95°.

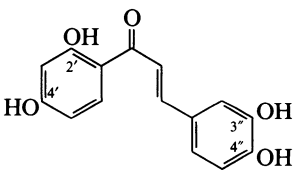
Grassman, W. *et al*, *Chem. Ber.*, 1956, **89**, 2523.
Cunningham, J. *et al*, *J. Chem. Soc.*, 1963, 2875 (*struct*, *synth*, *pmr*)
Grassman, W. *et al*, *J. Chem. Soc.*, 1965, 4579 (*isol*, *struct*)
Andrews, D.H. *et al*, *Can. J. Chem.*, 1968, **46**, 2525 (*isol*, *uv*)
Harper, S.H. *et al*, *J. Chem. Soc. C*, 1969, 1109 (*isol*)
Banks, H.J. *et al*, *Aust. J. Chem.*, 1971, **24**, 2427 (*deriv*)
Reimann, G., *Justus Liebigs Ann. Chem.*, 1971, **750**, 109 (*synth*)
Manners, G.D. *et al*, *Phytochemistry*, 1971, **10**, 607 (*occur*, *isol*, *uv*)
Nakajima, K. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 3050 (*isol*)
Hata, K. *et al*, *Chem. Pharm. Bull.*, 1979, **27**, 984 (*isol*)
Inamori, Y. *et al*, *Chem. Pharm. Bull.*, 1984, **32**, 213 (*props*, *pharmacol*)
Juneja, R.K. *et al*, *Phytochemistry*, 1985, **24**, 321 (*deriv*)

1-(2,4-Dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)-2-propen-1-one, 9CI D-80362

Updated Entry replacing D-20298

2′,3,4,4′-Tetrahydroxychalcone. ***Butein***

[21849-70-7]



$C_{15}H_{12}O_5$ M 272.257

(E)-form [487-52-5]
Constit. of *Dalbergia stevensonii* and *Dahlia variabilis*, *Butea frondosa*, *Coreopsis* spp., *Cosmos sulphureus* and others. Orange-yellow cryst. + $1H_2O$ (EtOH aq.). Mp 198°, Mp 213-215°.

Tetra-Ac: Mp 129-131°.

3-O-β-D-Glucopyranoside: [30382-19-5]. ***Monospermoside***
$C_{21}H_{22}O_{10}$ M 434.399
Constit. of the flowers of *Butea monosperma*. Yellow cryst. (MeOH aq.). Mp 194-195°.

4″-O-β-D-Glucopyranoside: [499-29-6]. ***Coreopsin.*** *Choreopsin*
$C_{21}H_{22}O_{10}$ M 434.399
Obt. from flowers of *Cosmos sulphureus*, *C. gigantea*, *Bidens frondosa* and other spp. Yellow needles (EtOH aq.). Mp 190-195° dec.

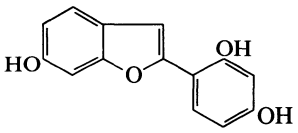
3′,4″-Di-O-β-D-glucopyranoside: ***Isobutrin.*** *Isobutyroin*
$C_{27}H_{32}O_{15}$ M 596.541
Isol. from flowers of *B. frondosa*. Bright-yellow cryst. (MeOH). Mp 190-191° dec. (sinters at 155°).

3″-Me ether: [34000-39-0]. *1-(2,4-Dihydroxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)-2-propen-1-one, 9CI. 2′,4,4′-Trihydroxy-3-methoxychalcone.* ***Homobutein***
$C_{16}H_{14}O_5$ M 286.284
Isol. from Subterranean clover *Trifolium subterraneum*. Mp 210-211°.

Price, J.R. *et al*, *J. Chem. Soc.*, 1939, 1017 (*isol, struct*)
Geissman, T.A., *J. Am. Chem. Soc.*, 1941, **63**, 2689; 1942, **64**, 1704 (*isol, deriv*)
Burkhart, W. *et al*, *Justus Liebigs Ann. Chem.*, 1942, **550**, 146 (*synth*)
Shimokoriyama, M., *J. Am. Chem. Soc.*, 1953, **75**, 1900 (*isol, deriv*)
Puri, B. *et al*, *J. Chem. Soc.*, 1955, 1589 (*Isobutrin*)
Wong, E. *et al*, *Phytochemistry*, 1968, **7**, 2123 (*Homobutein*)
Gupta, S.R. *et al*, *Phytochemistry*, 1970, **9**, 2231 (*Monospermoside*)
Saito, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2274 (*cryst struct*)
Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985, nos. 494, 495 (*occur, bibl*)

2-(2,4-Dihydroxyphenyl)-6-hydroxybenzofuran D-80363

Updated Entry replacing V-20015
4-(6-Hydroxy-2-benzofuranyl)-1,3-benzenediol, 9CI
[67736-22-5]



$C_{14}H_{10}O_4$ M 242.231
Isol. from heartwood of *Lespedeza cyrtobotrya*. Brownish needles. Mp 207-208°.

Tri-Ac: Mp 154-156°.

2′-Me ether: [74048-90-1]. *6-Hydroxy-2-(4-hydroxy-2-methoxyphenyl)benzofuran. 6-Demethylvignafuran*
$C_{15}H_{12}O_4$ M 256.257
Constit. of *Anthyllis vulneraria*, *Coronilla emerus* and *Tetragonolobus maritimus*leaves.

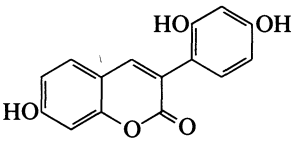
2′,6-Di-Me ether: [57800-41-6]. *2-(4-Hydroxy-2-methoxyphenyl)-6-methoxybenzofuran.* ***Vignafuran***
$C_{16}H_{14}O_4$ M 270.284
Constit. of leaves of *Vignia unguiculata* infected with *Colletotrichum lindenuthianium* and of *Lablab niger*. Phytoalexin. Glass.

2′,6-Di-Me ether, Ac: [57800-42-7].
Needles (MeOH). Mp 94-94.5°.

Preston, N.W. *et al*, *Phytochemistry*, 1975, **14**, 1843 (*isol, struct, uv, ms, pmr, synth, Vignafuran*)
Duffley, R.P. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1977, 802 (*synth, pmr, uv*)
Ingham, J.L. *et al*, *Phytochemistry*, 1978, **17**, 535; 1980, **19**, 289 (*Demethylvignafuran*)
Miyase, T. *et al*, *Chem. Pharm. Bull.*, 1981, **29**, 2205 (*isol, uv, ms*)

3-(2,4-Dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran-2-one D-80364

3-(2,4-Dihydroxyphenyl)-7-hydroxycoumarin

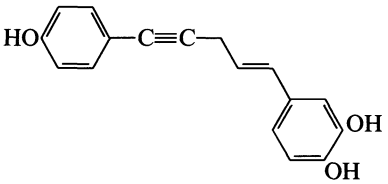


$C_{15}H_{10}O_5$ M 270.241

4′-Me ether: [54300-95-7]. *7-Hydroxy-3-(2-hydroxy-4-methoxyphenyl)coumarin. 2′,7-Dihydroxy-4′-methoxy-3-phenylcoumarin*
$C_{16}H_{12}O_5$ M 284.268
Isol. from heartwood of *Dalbergia olivieri*. Yellow rhombs (EtOH aq.). Mp 258-260°.

Donnelly, D.M.X. *et al*, *Phytochemistry*, 1974, **13**, 2587 (*isol, uw, pmr, struct*)

1-(3,4-Dihydroxyphenyl)-5-(4-hydroxyphenyl)-1-penten-4-yne D-80365

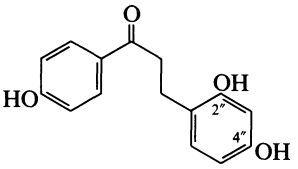


$C_{20}H_{20}O_3$ M 308.376
Constit. of *Hypoxis rooperi*.

Drewes, S.E. *et al*, *Phytochemistry*, 1989, **28**, 153.

3-(2,4-Dihydroxyphenyl)-1-(4-hydroxyphenyl)-1-propanone D-80366

2,4,4′-Trihydroxydihydrochalcone



$C_{15}H_{14}O_4$ M 258.273

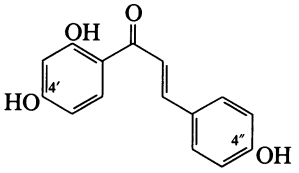
2″-Me ether: [116384-24-8]. *3-(4-Hydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone.* ***Loureirin C***
$C_{16}H_{16}O_4$ M 272.300
Constit. of *Dracaena loureiri*. Yellow foam. Mp 157-158°.

2″,-4″-Di-Me ether: [119425-89-7]. *3-(2,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone.* ***Loureirin A***
$C_{17}H_{18}O_4$ M 286.327
Constit. of *D. loureiri*. Cryst. Mp 124°.

Meksuriyen, D. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1129 (*isol, pmr, cmr*)

1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one D-80367

2′,4,4′-Trihydroxychalcone. ***Isoliquiretigenin***



$C_{15}H_{12}O_4$ M 256.257

Isol. from *Dahlia variabilis*, also from *Pterocarpus* spp., *Robinia pseudoacacia, Cicer arietinum, Glycyrrhiza uralensis, Pterocarbus indicus* and other leguminosae. Yellow cryst. (EtOH aq.). Mp 200-204°.

4′-O-β-D-Glucopyranoside: [59122-93-9]. ***Neoisoliquiritin***
$C_{21}H_{22}O_9$ M 418.399
Isol. from *G. glabra, G. uralensis, Cicer arietinum* and *Trifolium subterraneum*. Yellow needles (EtOH). Mp 230-232° (217-218°). $[\alpha]_D^{18}$ −61.5° (c, 0.5 in EtOH).

4″-O-β-D-Glucopyranoside: ***Isoliquiritin.*** *Isoliquiritoside*
$C_{21}H_{22}O_9$ M 418.399
Isol. from roots of *G. glabra* and from *D.* spp. Mp 185-186° dec.

4′-O-Glucosylglucoside:
$C_{27}H_{32}O_{14}$ M 580.541
Isol. from *Dahlia variabilis* and *Ulex europaeus*. λ_{max} 242, 372 nm (95% EtOH).

4″-O-[β-D-Glucopyranosyl(1→2)-β-D-apioside]: ***Liquiraside***
$C_{26}H_{30}O_{13}$ M 550.515
Isol. from *G. glabra* and *G. uralensis*. Gold cryst. (EtOH aq.). Mp 150-151°. $[\alpha]_D^{18}$ −125° (c, 0.8 in EtOH).

4′-O-Glucopyranosylglucopyranoside, 4″-O-glucopyranoside:
$C_{33}H_{42}O_{19}$ M 742.683
Isol. from *U. europaeus*. λ_{max} 237, 361 nm (95% EtOH).

4′-O-(Rhamnopyranosylglucopyranoside):
Rhamnoisoliquiritin
$C_{27}H_{32}O_{13}$ M 564.542
Isol. from liquorice root. Mp 127°.

O⁴′-Me: ***2′,4-Dihydroxy-4′-methoxychalcone***
$C_{16}H_{14}O_4$ M 270.284
Isol. from *Xanthorrhoeia australis*. Yellow needles (EtOH aq.). Mp 172-176°.

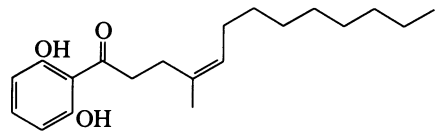
4′-O-α-L-Rhamnopyranoside: [78795-34-3].
$C_{27}H_{32}O_{13}$ M 564.542
Isol. from *Viburnum cortinifolium*. Yellow needles (MeOH aq.). Mp 60-63°.

[5041-81-6, 23141-04-0, 27233-96-1]

Geissman, T.A. *et al, J. Am. Chem. Soc.*, 1946, **68**, 697 (*bibl*)
Bate-Smith, E.C. *et al, J. Chem. Soc.*, 1953, 2183 (*isol*)
Duewell, H., *J. Chem. Soc.*, 1954, 2562 (*isol, deriv*)
Harborne, J.B., *Phytochemistry*, 1962, **1**, 203 (*glycosides*)
Litvinenko, V.I. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **155**, 600; 1966, **169**, 347 (*Neoisoliquiritin, Liquiraside*)
Kubota, T. *et al, Nippon Kagaku Zasshi* (*Jpn. J. Chem.*), 1966, **87**, 1201; *CA*, **66**, 94951y (*synth*)
Wong, E. *et al, Phytochemistry*, 1968, **7**, 2123 (*isol*)
Winger, G. *et al, Biochemistry*, 1969, **8**, 2067 (*synth*)
Van Hulle, C. *et al, Planta Med.*, 1971, **20**, 278 (*Rhamnoisoliquiritin*)
Markham, K.R. *et al, Tetrahedron*, 1976, **32**, 2607 (*cmr*)
Srivastava, S. *et al, Indian J. Chem., Sect. B*, 1981, **20**, 347 (*isol, deriv, uv*)
Maurya, R. *et al, J. Nat. Prod.* (*Lloydia*), 1984, **47**, 179 (*isol*)

1-(2,6-Dihydroxyphenyl)-4-methyl-4-tridecen-1-one D-80368

[119736-94-6]



$C_{20}H_{30}O_3$ M 318.455

(Z)-form

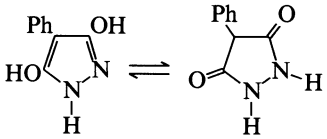
Constit. of *Horsfieldia glabra*. Cryst. (MeOH). Mp 42-44°.

Pinto, M.M.M. *et al, Phytochemistry*, 1988, **27**, 3988.

3,5-Dihydroxy-4-phenylpyrazole D-80369

1,2-Dihydro-5-hydroxy-4-phenyl-3H-pyrazol-3-one, 9CI. 4-Phenyl-3,5-pyrazolediol

[106367-54-8]



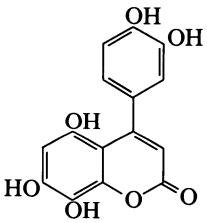
$C_9H_8N_2O_2$ M 176.174

Several other tautomers possible including zwitterions. In neutral solvs. the diol form appearsto predominate with extensive ionisation to the anion in polar solvs. Cryst. (THF). Mp 229°. pK_{a1} 3.70, pK_{a2} 12.71 (H_2O).

Zvilichovsky, G. *et al, J. Org. Chem.*, 1982, **47**, 295 (*synth, uv*)
Zvilichovsky, G. *et al, J. Heterocycl. Chem.*, 1988, **25**, 1307 (*tautom*)

4-(3,4-Dihydroxyphenyl)-5,7,8-trihydroxycoumarin D-80370

3′,4′,5,7,8-Pentahydroxyneoflavone



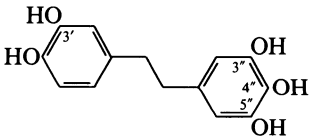
$C_{15}H_{10}O_7$ M 302.240

5,7-Di-Me ether: 4-(3,4-Dihydroxyphenyl)-8-hydroxy-5,7-dimethoxycoumarin. 3′,4′,8-Trihydroxy-5,7-dimethoxyneoflavone
$C_{17}H_{14}O_7$ M 330.293
Constit. of *Coutarea hexandra*.

D'Agostino, M. *et al, Phytochemistry*, 1989, **28**, 1773.

1-(3,4-Dihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethane D-80371

5-[2-(3,4-Dihydroxyphenyl)ethyl]-1,2,3-benzenetriol



$C_{14}H_{14}O_5$ M 262.262

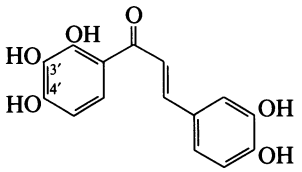
3″,4″,5″-Tri-Me ether: [116518-76-4]. *1-(3,4-Dihydroxyphenyl)-2-(3,4,5-trimethoxyphenyl)ethane.* ***Combretastatin B3***
$C_{17}H_{20}O_5$ M 304.342
Constit. of *Combretum caffrum*. Powder (EtOH/Et_2O). Mp 113-115°.

3′,3″,4″,5″-Tetra-Me ether: 1-(4-Hydroxy-3-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)-ethane. ***Crepidatin***
$C_{18}H_{22}O_5$ M 318.369
Constit. of *Dendrobium crepidatum*. Cryst. (EtOAc/pet. ether). Mp 99°.

Pettit, G.R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 517.
Majumder, P.L. *et al*, *Phytochemistry*, 1989, **28**, 1986.

3-(3,4-Dihydroxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one D-80372

2′,3,3′,4,4′-Pentahydroxychalcone



$C_{15}H_{12}O_6$ M 288.256

3′-Me ether: [6542-59-2]. *1-(2,4-Dihydroxy-3-methoxyphenyl)-3-(3,4-dihydroxyphenyl)-2-propen-1-one. 2′,3,4,4′-Tetrahydroxy-3′-methoxychalcone.* ***Lanceoletin***
$C_{16}H_{14}O_6$ M 302.283
Rare chalcone present in floral tissues of some Compositae.

3′-Me ether, tetra-Ac: Pale-yellow prisms (MeOH). Mp 162-166°.

3′-Me ether, 4′-O-β-D-glucopyranoside: [64181-95-9]. ***Lanceolin***†
$C_{22}H_{24}O_{11}$ M 464.425
Isol. from *Coreopsis lanceolata*.

Shinokoriyama, M. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 1900 (*isol, struct*)
Nicholls, K.W. *et al*, *Phytochemistry*, 1979, **18**, 1076 (*isol*)
Crawford, D.J. *et al*, *Am. J. Bot.*, 1983, **70**, 355; *CA*, **98**, 212856g (*occur*)

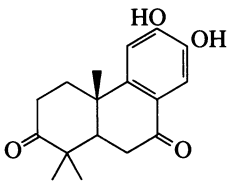
ent-3β,14α-Dihydroxy-7,9(11),15-pimaratriene-2,12-dione D-80373

Yucalexin P-15

[119626-52-7]
$C_{20}H_{26}O_4$ M 330.423
Constit. of cassava roots (*Manihot esculenta*).

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

12,13-Dihydroxy-8,11,13-podocarpatriene-3,7-dione D-80374



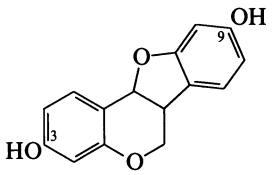
$C_{17}H_{20}O_4$ M 288.343

Di-Me ether: [119269-83-9]. *12,13-Dimethoxy-8,11,13-podocarpatriene-3,7-dione.* ***Methyl nimbionone***
$C_{19}H_{24}O_4$ M 316.396
Constit. of *Azadirachta indica*. Needles (hexane). Mp 116-119°.

Ara, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1054.

3,9-Dihydroxypterocarpan D-80375

Updated Entry replacing D-60373
Demethylmedicarpin
[61135-91-9]



$C_{15}H_{12}O_4$ M 256.257
Isol. from *Albizia prozera, Erythrina crista-galli, E. sandwicensis, Melilotus alba, Pachyrrhizus erosus, Phaseolus vulgaris, Psophocarpus tetragonolobus* and *Trifolium repens*.Fungal metab. of Medicarpin. Pale yellow amorph. powder.

Di-Ac: Needles. Mp 122°. $[\alpha]_D$ +126° (c, 0.25 in $CHCl_3$).

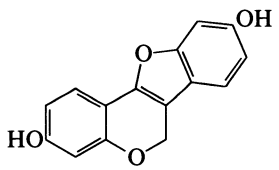
3-Me ether: [38822-00-3]. *9-Hydroxy-3-methoxypterocarpan.* ***Isomedicarpin***
$C_{16}H_{14}O_4$ M 270.284
Constit. of *Psophocarpus tetragonolobus*. Cryst. Mp 106°. $[\alpha]_D^{18}$ −201° ($CHCl_3$).

McMurry, T.B.H. *et al*, *Phytochemistry*, 1972, **11**, 3283 (*synth*)
Deshpande, V.H. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 201 (*isol*)
Preston, N.W. *et al*, *Phytochemistry*, 1977, **16**, 2044 (*Isomedicarpin*)
Ingham, J.L. *et al*, *Phytochemistry*, 1980, **19**, 1203 (*Isomedicarpin*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Prasad, A.V.K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1986, 1561 (*synth*)

3,9-Dihydroxypterocarpene D-80376

6H-Benzofuro[3,2-c][1]benzopyran-3,9-diol, 9CI. ***Anhydroglycinol***

[67685-22-7]



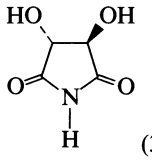
$C_{15}H_{10}O_4$ M 254.242
Isol. from heartwood of *Lespedeza cyrtobotrya*; phytoalexin from *Tetragonolobus maritimus* R1. Cryst. (MeOH/$CHCl_3$). Mp 207-209° dec.

Di-Me ether: [1433-08-5]. *3,9-Dimethoxypterocarpene. 3,9-Dimethoxy-6H-benzofuro*[3,2-c][1]*benzopyran, 9CI.* ***Anhydrovariabilin***
$C_{17}H_{14}O_4$ M 282.295
Isol. from heartwoods of *Dalbergia decipularis* and *Swartzia madagascariensis*. Prisms (EtOH). Mp 116° (110-112°).

Bowyer, W.J. *et al*, *J. Chem. Soc.*, 1964, 4212 (*synth, deriv*)
Harper, S.H. *et al*, *J. Chem. Soc. C*, 1969, 1109 (*isol, deriv*)
De Alencar, R. *et al*, *Phytochemistry*, 1972, **11**, 1517 (*isol, deriv*)
Miyase, T. *et al*, *Chem. Pharm. Bull.*, 1980, **28**, 1172 (*isol, uv, ir, pmr*)

3,4-Dihydroxy-2,5-pyrrolidinedione, 9CI D-80377

Tartrimide, 8CI. 2,3-Dihydroxysuccinimide



(3*R*,4*R*)-*form*

$C_4H_5NO_4$ M 131.088

(*3R,4R*)-*form* [18366-18-2]
Mp 200° dec. (205-206°). $[\alpha]_D^{20}$ +202° (c, 0.5 in H_2O).

Di-tert-*butyl ether:* [117237-94-2].
$C_{12}H_{21}NO_4$ M 243.302
Cryst. (toluene/hexane). Mp 154°. $[\alpha]_D^{20}$ +205° (c, 1 in $CHCl_3$).

N-*Benzyl:* [19728-93-9].
Cryst. (H_2O). Mp 196-198°. $[\alpha]_D^{25}$ +126° (MeOH).

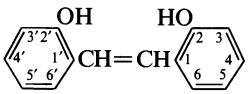
Dave, H.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 743 (*synth, cd*)
Wong, C.M. *et al*, *Can. J. Chem.*, 1968, **46**, 3091 (*deriv*)
Poloński, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 629 (*synth, ir, uv, pmr, cd*)

2,2′-Dihydroxystilbene D-80378

Updated Entry replacing B-40108

2,2′(1,2-Ethenediyl)bisphenol, 9CI. 2,2′-Stilbenediol, 8CI. 1,2-Bis(2-hydroxyphenyl)ethylene

[4752-75-4]



$C_{14}H_{12}O_2$ M 212.248

(*E*)-*form* [18221-50-6]
Needles (EtOH). Mp 197°.

Di-Ac: [51042-12-7].
$C_{18}H_{16}O_4$ M 296.322
Mp 141-142°.

Di-Me ether: [20516-15-8].
$C_{16}H_{16}O_2$ M 240.301
Mp 136°.

(*Z*)-*form*
Mp 95°.

Dibenzoyl:
$C_{28}H_{20}O_4$ M 420.464
Mp 107-108°.

Buu-Hoï, Ng.Ph. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 955 (*synth*)
Lapkin, I.I. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 1968 (*synth*)
Tirado-Rives, J. *et al*, *J. Org. Chem.*, 1984, **49**, 1627 (*synth, pmr, cmr, ir, ms, uv, cryst struct*)

2,4′-Dihydroxystilbene D-80379

2-[2-(4-Hydroxyphenyl)ethenyl]phenol, 9CI. 2,4′-Stilbenediol. 1-(2-Hydroxyphenyl)-2-(4-hydroxyphenyl)ethylene

$C_{14}H_{12}O_2$ M 212.248

(*E*)-*form* [110983-43-2]
Mp 193-194°.

Mylona, A. *et al*, *J. Chem. Res.* (*S*), 1986, 433 (*synth, ir, uv*)

2,5-Dihydroxystilbene D-80380

2-(2-Phenylethenyl)-1,4-benzenediol, 9CI. 2,5-Stilbenediol. 1-(2,5-Dihydroxyphenyl)-2-phenylethylene

$C_{14}H_{12}O_2$ M 212.248

(*E*)-*form* [34701-58-1]
Mp 165-166°. $Bp_{0.001}$ 150-155° subl.

(*Z*)-*form* [34701-63-8]
Cryst. (Et_2O). Mp 90-92°.

Bruce, J.M. *et al*, *J. Chem. Soc. C*, 1971, **22**, 3749 (*synth, ir, uv, pmr*)

3,3′-Dihydroxystilbene D-80381

3,3′-(1,2-Ethenediyl)bisphenol, 9CI. 1,2-Bis(3-hydroxyphenyl)ethylene. 3,3′-Stilbenediol

[70709-65-8]

$C_{14}H_{12}O_2$ M 212.248
Needles (hexane). Mp 111-112°.

Hata, K. *et al*, *Chem. Pharm. Bull.*, 1979, **27**, 984 (*synth, ir, pmr*)

3,4-Dihydroxystilbene D-80382

4-(2-Phenylethenyl)-1-2-benzenediol, 9CI. 3,4-Stilbenediol. 1-(3,4-Dihydroxyphenyl)-2-phenylethylene

$C_{14}H_{12}O_2$ M 212.248

(*E*)-*form* [19826-29-0]
Platelets (Me_2CO/C_6H_6). Mp 168-169°.

Gorham, J. *et al*, *Phytochemistry*, 1980, **19**, 2059.
Donnelly, D.M.X. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 2719 (*synth, ir, uv, pmr*)

3,4′-Dihydroxystilbene D-80383

3-[2-(4-Hydroxyphenyl)ethenyl]phenol, 9CI. 3,4′-Stilbenediol. 1-(3-Hydroxyphenyl)-2-(4-hydroxyphenyl)ethylene

[62574-04-3]

$C_{14}H_{12}O_2$ M 212.248
Isolated from roots of *Hydrangea macrophylla*.

[63877-76-9]

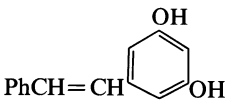
Gorham, J., *Phytochemistry*, 1977, **16**, 249 (*isol*)

3,5-Dihydroxystilbene D-80384

Updated Entry replacing P-01174

5-(2-Phenylethenyl)-1,3-benzenediol, 9CI. 1-(3,5-Dihydroxyphenyl)-2-phenylethylene. 5-Styrylresorcinol. ***Pinosylvin***

[102-61-4]



$C_{14}H_{12}O_2$ M 212.248

(*E*)-*form* [22139-77-1]
Constit. of *Pinus* spp. and *Dalbergia sissoo*. Shows fungistatic props. Needles (AcOH). Mp 155.5-156°.
▷ WJ5580000.

Di-Ac:
$C_{18}H_{16}O_4$ M 296.322
Mp 100-101°.

Mono-Me ether: [5150-38-9]. *3-Methoxy-5-(2-phenylethenyl)phenol, 9CI. 3-Hydroxy-5-methoxystilbene. 5-Methoxy-3-stilbenol*
$C_{15}H_{14}O_2$ M 226.274
Isol. from wood of many *P.* spp. Cryst. Mp 122-123°.

Di-Me ether: [21956-56-9].
$C_{16}H_{16}O_2$ M 240.301
Isol. from wood of *P. palustris*, *P. griffithii*, *P. formosana* and other *P.* spp. Prisms (MeOH). Mp 56-57°.

(*Z*)-*form* [106325-78-4]

Di-Me ether: [21956-55-8].
Isol. from Jack pine (*P. banksiana*). $Bp_{0.02}$ 123°.

Erdtmann, H., *Justus Liebigs Ann. Chem.*, 1939, **539**, 116 (*isol, struct*)
Cox, R.F.B., *J. Am. Chem. Soc.*, 1940, **62**, 3512 (*isol, struct*)
Liebherr, E. *et al*, *Ber.*, 1941, **74**, 869 (*synth*)
Erdtmann, H. *et al*, *Phytochemistry*, 1966, **5**, 927 (*isol*)
Rowe, J.W. *et al*, *Phytochemistry*, 1969, **8**, 235 (*isol, derivs*)
Bachelor, F.W. *et al*, *Can. J. Chem.*, 1970, **48**, 1554 (*synth*)
Cardona, L. *et al*, *Tetrahedron*, 1986, **42**, 2725 (*synth, pmr, cmr*)

4,4′-Dihydroxystilbene D-80385

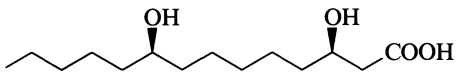
Updated Entry replacing B-01588
4,4′-(1,2-Ethenediyl)bisphenol, 9CI. 4,4′-Stilbenediol, 8CI. 1,2-Bis(4-hydroxyphenyl)ethylene
[659-22-3]
$C_{14}H_{12}O_2$ M 212.248
Needles (AcOH). Mp 293-294° (284°).

Di-Ac:
$C_{18}H_{16}O_4$ M 296.322
Mp 213°.

Di-Me ether: [4705-34-4].
$C_{16}H_{16}O_2$ M 240.301
Mp 214-215°. Sublimes.

Laarhoven, W.H., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1961, **80**, 775 (*synth*)
Sieber, R.W., *Justus Liebigs Ann. Chem.*, 1969, **730**, 31 (*synth*)

3,9-Dihydroxytetradecanoic acid D-80386

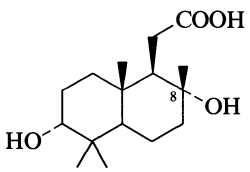


(3*R*,9*R*)-*form*

$C_{14}H_{28}O_4$ M 260.373
(3R,9R)-form
Me ester: [115482-43-4].
$C_{15}H_{30}O_4$ M 274.400
Solid. Mp 57-59°. $[\alpha]_D^{27}$ −10.55° (c, 1.45 in $CHCl_3$).

Schreiber, S.L. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6210 (*synth, pmr, cmr, ms, ir*)

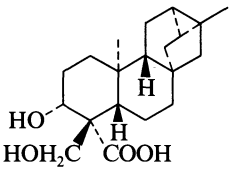
3,8-Dihydroxy-13,14,15,16-tetranor-12-labdanoic acid D-80387



$C_{16}H_{28}O_4$ M 284.395
(3α,8α)-form
*8-Ac, Me ester: Methyl 8α-acetoxy-3α-hydroxy-*13,14,15,16-*tetranorlabdan-*12-*oate*
$C_{19}H_{32}O_5$ M 340.459
Constit. of *Salvia aethiopis*. Gum. $[\alpha]_D$ −0.79° (c, 1.05 in $CHCl_3$).

Gonzalez, M.S. *et al*, *Tetrahedron*, 1989, **45**, 3575.

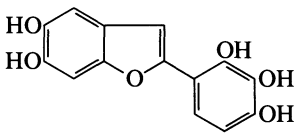
ent-3β,18-Dihydroxy-19-trachylobanoic acid D-80388



$C_{20}H_{30}O_4$ M 334.455
Constit. of *Jungermannia exsertifolia* subsp. *cordifolia*.
Me ester: Cryst. (hexane). Mp 134-135°. $[\alpha]_D$ −60.8° (c, 0.75 in $CHCl_3$).

Harrison, L.J. *et al*, *Phytochemistry*, 1989, **28**, 1533.

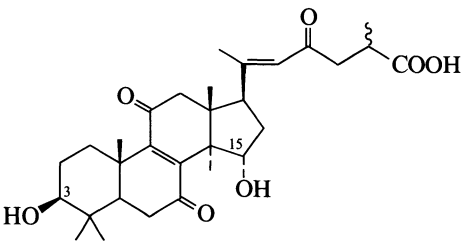
5,6-Dihydroxy-2-(2,3,4-trihydroxyphenyl)benzofuran D-80389



$C_{14}H_{10}O_6$ M 274.229
3′-Me, 5,6-methylene ether: [79295-81-1]. *2-(2,4-Dihydroxy-3-methoxyphenyl)-5,6-methylenedioxybenzofuran. 5-Furo[2,3-*f*]-*1,3*-benzodioxol-*6*-yl-*2*-methoxy-*1,3*-benzenediol, 9CI.* ***Sophorafuran A***
$C_{16}H_{12}O_6$ M 300.267
Isol. from roots of *Sophora franchetiana*. Needles (C_6H_6). Mp 145-146°.

Komatsu, M. *et al*, *Chem. Pharm. Bull.*, 1981, **29**, 2069 (*isol, uv, ms, pmr, cmr, struct*)

3,15-Dihydroxy-7,11,23-trioxo-8,20-lanostadien-26-oic acid D-80390

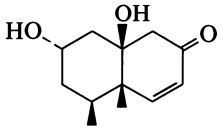


$C_{30}H_{42}O_7$ M 514.658
(3β,15α,20E)-form [120462-49-9] ***Ganoderenic acid I***
Constit. of *Ganoderma applantum*.
Me ester: $[\alpha]_D^{23}$ +96° (c, 0.2 in EtOH).
3-Ketone: [120481-73-4]. *15α-Hydroxy-*3,7,11,23-*tetraoxo-*8,20E-*lanostadien-*26-*oic acid.* ***Ganoderenic acid G***
$C_{30}H_{40}O_7$ M 512.642
Constit. of *G. applantum*. $[\alpha]_D^{23}$ +189° (c, 0.2 in EtOH).
15-Ketone: [120462-48-8]. *3β-Hydroxy-*7,11,15,23-*tetraoxo-*8,20E-*lanostadien-*26-*oic acid.* ***Ganoderenic acid H***
$C_{30}H_{40}O_7$ M 512.642
Constit. of *G. applantum*.
15-Ketone, Me ester: $[\alpha]_D^{23}$ +61° (c, 0.2 in EtOH).
3,15-Diketone: [120462-47-7]. *3,7,11,15,23-Pentaoxo-8,20*E-*lanostadien-*26-*oic acid.* ***Ganoderenic acid F***
$C_{30}H_{38}O_7$ M 510.626
Constit. of *G. applantum*. $[\alpha]_D^{23}$ +93° (c, 0.2 in EtOH).

Nishitoba, T. *et al*, *Phytochemistry*, 1989, **28**, 193.

2,10-Dihydroxy-11,12,13-trisnor-6-eremophilen-8-one D-80391

2,10-Dihydroxyondetianone



$C_{12}H_{18}O_3$ M 210.272

(2α,10β)-form

Constit. of *Ondetia linearis*. Cryst. Mp 148°. $[\alpha]_D^{24}$ +27° (c, 0.23 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

1,11-Dihydroxy-6-undecanone, 9CI D-80392

[116288-12-1]

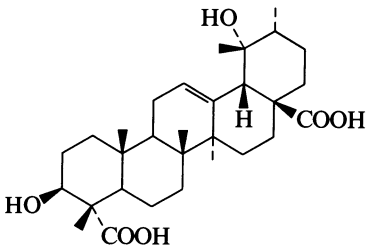
$HOCH_2(CH_2)_4CO(CH_2)_4CH_2OH$

$C_{11}H_{22}O_3$ M 202.293

Solid. Mp 58.5°.

Momenteau, M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 283 (*synth, pmr*)

3,19-Dihydroxy-12-ursene-23,28-dioic acid D-80393



$C_{30}H_{46}O_6$ M 502.690

(3β,19α)-form

Rotundioic acid

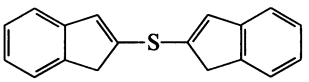
Constit. of *Ilex rotunda*. Cryst. (MeOH). Mp 295-298° dec. $[\alpha]_D$ +50° (MeOH).

Nakatani, M. *et al*, *Phytochemistry*, 1989, **28**, 1479.

Di-2-indenyl sulfide D-80394

*2,2′-Thiobis-1*H*-indene*

[115679-49-7]



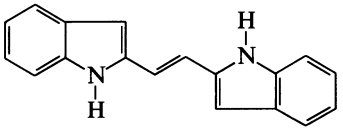
$C_{18}H_{14}S$ M 262.375

Mp 96°.

Baierweck, P. *et al*, *Chem. Ber.*, 1988, **121**, 2195 (*synth, pmr, cmr*)

1,2-Di-2-indolylethylene D-80395

*2,2′-(1,2-Ethenediyl)bis-1*H*-indole, 9CI*



$C_{18}H_{14}N_2$ M 258.322

(E)-form [115983-53-4]

Cream cryst. (EtOAc). Mp >300° (resinifies above 280°).

N,N′-Di-Me: [115983-54-5].

$C_{20}H_{18}N_2$ M 286.376

Yellow needles (EtOAc). Mp 251°.

Capuano, L. *et al*, *Chem. Ber.*, 1988, **121**, 2259 (*synth, pmr, uv*)

2,3-Diiodobenzoic acid, 9CI, 8CI D-80396

Updated Entry replacing D-05161

$C_7H_4I_2O_2$ M 373.916

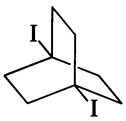
Cryst. (EtOH). Mp 183-185° (178-181°).

Twiss, D. *et al*, *J. Org. Chem.*, 1950, **15**, 496 (*synth*)

Newman, M.S. *et al*, *J. Org. Chem.*, 1971, **36**, 1398 (*synth, pmr*)

1,4-Diiodobicyclo[2.2.2]octane D-80397

[10364-05-3]



$C_8H_{12}I_2$ M 361.992

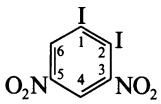
Cryst. (hexane/EtOH). Mp 239-240°.

McKinley, J.W. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 2030 (*synth, pmr*)

Zimmerman, H.E. *et al*, *J. Org. Chem.*, 1980, **45**, 3933 (*synth*)

Adcock, W. *et al*, *J. Org. Chem.*, 1988, **53**, 5259 (*synth*)

1,2-Diiodo-3,5-dinitrobenzene D-80398



$C_6H_2I_2N_2O_4$ M 419.902

Yellow cryst. (CCl_4/pet. ether). Mp 110°.

Deorha, D.S. *et al*, *J. Indian Chem. Soc.*, 1965, **42**, 101 (*synth*)

1,2-Diiodo-4,5-dinitrobenzene D-80399

[29270-47-1]

$C_6H_2I_2N_2O_4$ M 419.902

Pale yellow needles (AcOH). Mp 183-184°.

Deorha, D.S. *et al*, *J. Indian Chem. Soc.*, 1965, **42**, 101 (*synth*)

Arotsky, J. *et al*, *J. Chem. Soc. C*, 1970, 1480 (*synth, pmr*)

1,3-Diiodo-4,6-dinitrobenzene D-80400

[37923-51-6]

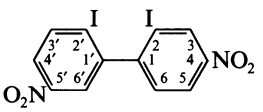
$C_6H_2I_2N_2O_4$ M 419.902

Mp 161-162°.

Siddalingaiah, K.S. *et al*, *Curr. Sci.*, 1972, **41**, 451 (*synth*)

Shamanna, D. *et al*, *Indian J. Chem.*, 1974, **12**, 510.

2,2′-Diiodo-4,5′-dinitrobiphenyl D-80401



$C_{12}H_6I_2N_2O_4$ M 495.999

Pale yellow prisms (EtOH). Mp 167-168°.

Baker, W. *et al*, *J. Chem. Soc.*, 1958, 2658 (*synth*)

2,2′-Diiodo-5,5′-dinitrobiphenyl D-80402

[61837-21-6]

$C_{12}H_6I_2N_2O_4$ M 495.999
Pale yellow cryst. (EtOH/Me_2CO). Mp 236-238°.

Dougherty, T.K. *et al*, *J. Org. Chem.*, 1983, **48**, 5273 (*synth, ir, pmr*)

2,2′-Diiodo-6,6′-dinitrobiphenyl D-80403

[17532-87-5]

$C_{12}H_6I_2N_2O_4$ M 495.999
Pale yellow prisms (C_6H_6). Mp 152-153°.

Iqbal, K. *et al*, *J. Chem. Soc. C*, 1967, 1690 (*synth, pmr*)

4,4′-Diiodo-3,3′-dinitrobiphenyl D-80404

$C_{12}H_6I_2N_2O_4$ M 495.999
Yellow needles (EtOH). Mp 151-152°.

Wirth, H.O. *et al*, *Makromol. Chem.*, 1964, **77**, 90 (*synth*)

1,12-Diiodododecane D-80405

Dodecamethylene diiodide

[24772-65-4]

$$ICH_2(CH_2)_{10}CH_2I$$

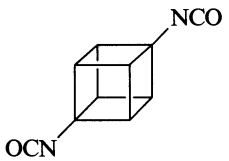
$C_{12}H_{24}I_2$ M 422.131
Platelets (EtOAc). Mp 41°. $Bp_{0.5}$ 192-198°.

Nineham, A.W., *J. Chem. Soc.*, 1953, 2601 (*synth*)
Ainscow, T.A. *et al*, *Tetrahedron*, 1987, **43**, 115 (*synth, pmr*)

1,4-Diisocyanatocubane D-80406

1,4-Diisocyanatopentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, 9CI

[116635-16-6]



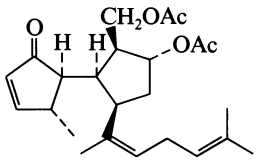
$C_{10}H_6N_2O_2$ M 186.170
Solid by subl. Mp 113-115°. Moisture sensitive, stable under N_2 in cold.

▷ Hazardous prepn., can explode.

Eaton, P.E. *et al*, *J. Org. Chem.*, 1988, **53**, 5353 (*synth, pmr, cmr, ir*)

Dilophus enone D-80407

[121961-78-2]

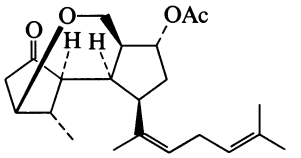


$C_{24}H_{34}O_5$ M 402.530
Constit. of alga *Dilophus okamurai*. Antifeedant. $[\alpha]_D$ −46.0° (c, 1.30 in $CHCl_3$).

Kurata, K. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1567.

Dilophus ether D-80408

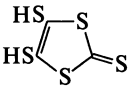
[121940-50-9]



$C_{22}H_{32}O_4$ M 360.492
Constit. of alga *Dilophus okamurai*. Antifeedant. $[\alpha]_D$ −69.0° (c, 0.860 in $CHCl_3$).

Kurata, K. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1567.

4,5-Dimercapto-1,3-dithiole-2-thione D-80409



$C_3H_2S_5$ M 198.379

Di-Na salt: [54995-24-3].
Crimson red solid. Fairly stable under Ar in dark.

Di-Me thioether: [49638-64-4].
$C_5H_6S_5$ M 226.432
Mp 99-100°.

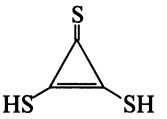
Di-Et thioether: [59065-21-3].
$C_7H_{10}S_5$ M 254.486
Mp 36.5-37°.

Dibenzyl thioether: [54995-25-4].
$C_{17}H_{14}S_5$ M 378.628
Mp 86°.

Wawzonek, S. *et al*, *J. Org. Chem.*, 1974, **39**, 511 (*synth, ir, raman, pmr, uv, ms*)
Steinecke, G. *et al*, *Z. Chem.*, 1975, **15**, 28 (*synth*)
Reuter, U. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **421**, 143 (*synth, deriv, ms, uv, pmr*)
Hartke, K. *et al*, *Chem. Ber.*, 1980, **113**, 1898 (*deriv, synth*)
Varma, S.K. *et al*, *Synthesis*, 1987, 837 (*synth*)

2,3-Dimercapto-2-propene-1-thione D-80410

Trithiodeltic acid



$C_3H_2S_3$ M 134.247

Di-Na salt: Beige solid. Mp >300°. Mesomeric.

Baum, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 1163 (*synth, cryst struct*)

3,4-Dimethoxybenzyl isothiocyanate D-80411

4-(Isothiocyanatomethyl)-1,2-dimethoxybenzene. Veratryl isothiocyanate

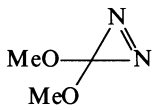
[14596-50-0]

$C_{10}H_{11}NO_2S$ M 209.268
Isol. from seeds of *Heliophila longifolia*. Viscous pale-yellow oil or cryst. Mp 22-24°. Bp 135-137°. n_D^{25} 1.5960.

Ettlinger, M.G. *et al*, *Acta Chem. Scand.*, 1966, **20**, 1778 (*isol, struct, synth*)

3,3-Dimethoxy-3*H*-diazirine, 9CI **D-80412**

[114980-39-1]

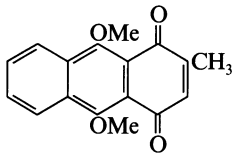


$C_3H_6N_2O_2$ M 102.093

Precursor for Dimethoxycarbene. Obt. as *ca* 0.7 M pentane soln.

Moss, R.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4443 (*synth, uw, use*)

9,10-Dimethoxy-2-methyl-1,4-anthraquinone **D-80413**



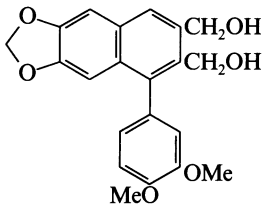
$C_{17}H_{14}O_4$ M 282.295

Constit. of *Tectonia grandis*. Yellow cryst.

Singh, P. *et al*, *Phytochemistry*, 1989, **28**, 1258.

1-(3,4-Dimethoxyphenyl)-2,3-bis(hydroxymethyl)-6,7-methylenedioxynaphthalene **D-80414**

[42923-60-4]



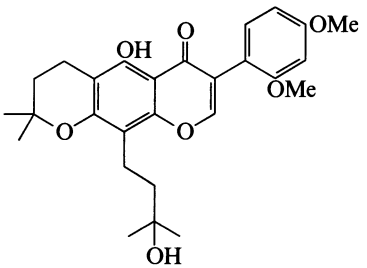
$C_{21}H_{20}O_6$ M 368.385

Constit. of *Jatropha gossypifolia*. Cryst. (C_6H_6/pet. ether). Mp 184°.

Das, B. *et al*, *Phytochemistry*, 1988, **27**, 3684.

7-(2,4-Dimethoxyphenyl)-3,4-dihydro-5-hydroxy-10-(3-hydroxy-3-methylbutyl)-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, 9CI **D-80415**

[78876-32-1]



$C_{27}H_{32}O_7$ M 468.546

Isol. from leaves of *Millettia pachycarpa*. Cryst. (pet. ether). Mp 150°.

Singhal, A.K. *et al*, *Phytochemistry*, 1981, **20**, 803 (*isol, uw, pmr, ms, struct*)

7-(3,4-Dimethoxyphenyl)-3,4-dihydro-5-hydroxy-10-(3-hydroxy-3-methylbutyl)-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,6-*b*′]dipyran-6-one, 9CI **D-80416**

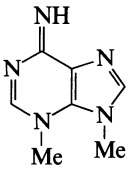
[78876-31-0]

$C_{27}H_{32}O_7$ M 468.546

Isol. from leaves of *Millettia pachycarpa*. Cryst. (EtOAc/pet. ether). Mp 140°.

Singhal, A.K. *et al*, *Phytochemistry*, 1981, **20**, 803 (*isol, uw, pmr, ms, struct*)

3,9-Dimethyladenine **D-80417**



$C_7H_9N_5$ M 163.182

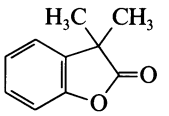
B,HCl: Prisms. Mp 281-282° dec.

B,HClO$_4$: Prisms (H_2O). Mp >300°. Other 3,9-dialkyladenines also prepd.

Fujii, T. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1504 (*synth, uw, pmr*)

3,3-Dimethyl-2(3*H*)-benzofuranone **D-80418**

[13524-76-0]



$C_{10}H_{10}O_2$ M 162.188

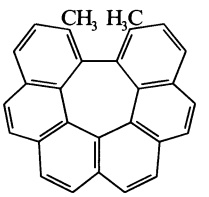
Liq. Bp_2 101-102°, $Bp_{0.4}$ 63°.

Gripenberg, J. *et al*, *Acta Chem. Scand.*, 1966, **20**, 1561 (*synth, uw, ir, pmr*)

Amyes, T.L. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6505 (*synth, ir, pmr, ms*)

7,8-Dimethylbenzo[*no*]naphtho[2,1,8,7-*ghij*]pleiadene, 9CI **D-80419**

1,16-Dehydro-2,15-dimethylhexahelicene



$C_{28}H_{18}$ M 354.450

(+)-***form***

Cryst. (C_6H_6/hexane). Mp 220-222°. $[\alpha]_D^{25}$ +1879° ($CHCl_3$).

(−)-***form***

Cryst. (C_6H_6/hexane). Mp 221-223°. $[\alpha]_D^{25}$ −1882° ($CHCl_3$).

(±)-***form*** [114417-96-8]

Yellow prisms (C_6H_6/hexane). Mp 226-228°.

[114324-63-9, 114417-92-4]

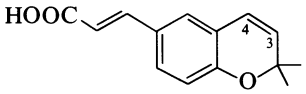
Yamamoto, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3578 (*synth, ir, pmr, uw, resoln, abs config*)

3-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid D-80420

Updated Entry replacing D-50601

2,2-Dimethylchromene-6-propenoic acid

[104387-05-5]



$C_{14}H_{14}O_3$ M 230.263

Constit. of *Baccharis* spp. Cryst. Mp 191-192°.

3,4-Dihydro: [12772-83-7]. *3-(3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid, 9CI.* ***Drupacin***

$C_{14}H_{16}O_3$ M 232.279

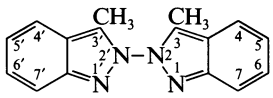
Isol. from fruits of *Psoralea drupacea*. Acicular cryst. (MeOH). Mp 205-206°.

Golovina, L.A. *et al*, *Khim. Prir. Soedin.*, 1973, **9**, 700; *Chem. Nat. Compd.*, 672 (*Drupacin*)

Labbe, C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1986, **49**, 517.

3,3′-Dimethyl-2,2′-biindazole D-80421

[113302-76-4]



$C_{16}H_{14}N_4$ M 262.313

Cryst. Mp 143-144°.

Cuevas, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 2055 (*synth, ir, ms, pmr, cmr*)

5,5′-Dimethyl-2,2′-biindazole D-80422

[113302-77-5]

$C_{16}H_{14}N_4$ M 262.313

Cryst. Mp 218.5-219.5°.

Cuevas, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 2055 (*synth, ir, ms, pmr, cmr*)

7,7′-Dimethyl-2,2′-biindazole D-80423

[113302-78-6]

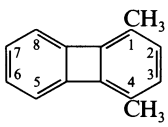
$C_{16}H_{14}N_4$ M 262.313

Cryst. Mp 165-166°.

Cuevas, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 2055 (*synth, ir, pmr, cmr, ms*)

1,4-Dimethylbiphenylene D-80424

[64472-47-5]



$C_{14}H_{12}$ M 180.249

Cryst. (EtOH). Mp 28°.

Hellwinkel, D. *et al*, *Justus Liebigs Ann. Chem.*, 1977, 1013 (*synth, pmr*)

1,5-Dimethylbiphenylene D-80425

[55277-56-0]

$C_{14}H_{12}$ M 180.249

Cryst. Mp 51-53°.

Campbell, C.D. *et al*, *J. Chem. Soc. C*, 1969, 742 (*synth*)

Wilcox, C.F. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 1914 (*synth*)

1,8-Dimethylbiphenylene D-80426

[36230-17-8]

$C_{14}H_{12}$ M 180.249

Pale yellow plates (MeOH). Mp 79-80°.

Picrate: Crimson needles (EtOH). Mp 126°.

Lothrop, W.C. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 1698 (*synth*)

Campbell, C.D. *et al*, *J. Chem. Soc. C*, 1969, 742 (*synth*)

Wilcox, C.F. *et al*, *J. Org. Chem.*, 1988, **53**, 4333; 1989, **54**, 2190 (*synth, pmr, cmr, bibl*)

2,3-Dimethylbiphenylene D-80427

[65350-34-7]

$C_{14}H_{12}$ M 180.249

Pale yellow cryst. (MeOH). Mp 111-112°.

Buckland, P.R. *et al*, *Tetrahedron*, 1977, **33**, 1797 (*synth, pmr*)

2,6-Dimethylbiphenylene D-80428

[2918-97-0]

$C_{14}H_{12}$ M 180.249

Pale yellow cryst. (EtOH). Mp 139-141°.

Hart, F.A. *et al*, *J. Chem. Soc.*, 1957, 3939 (*synth, uv*)

Campbell, C.D. *et al*, *J. Chem. Soc. C*, 1969, 742 (*synth*)

2,7-Dimethylbiphenylene D-80429

[4874-81-1]

$C_{14}H_{12}$ M 180.249

Pale yellow plates (EtOH). Mp 115°.

Picrate: Crimson needles (EtOH). Mp 110°.

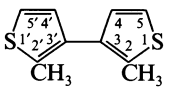
Lothrop, W.C., *J. Am. Chem. Soc.*, 1941, **63**, 1187 (*synth, deriv*)

Constantine, P.R. *et al*, *J. Chem. Soc. C*, 1966, 1767 (*synth, uv, pmr*)

Campbell, C.D. *et al*, *J. Chem. Soc. C*, 1969, 742 (*synth*)

2,2′-Dimethyl-3,3′-bithiophene, 9CI D-80430

[15940-57-5]



$C_{10}H_{10}S_2$ M 194.321

Bp_{17} 141-144°.

Gronowitz, S. *et al*, *Ark. Kemi*, 1967, **27**, 153 (*synth, pmr*)

Wiklund, E. *et al*, *Chem. Scr.*, 1973, **3**, 226 (*pmr*)

Gronowitz, S. *et al*, *Tetrahedron*, 1978, **34**, 587 (*synth*)

3,3′-Dimethyl-2,2′-bithiophene, 9CI D-80431

$C_{10}H_{10}S_2$ M 194.321

Liq. Bp_{25} 160-162°, Bp_{11} 131°.

Uhlenbroek, J.H. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1960, **79**, 1181 (*synth, uv*)

Gronowitz, S. *et al*, *Tetrahedron*, 1978, **34**, 587 (*synth, pmr*)

Cunningham, D.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1021 (*uv*)

Krische, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1476 (*synth, pmr*)

3,4′-Dimethyl-2,2′-bithiophene, 9CI D-80432

[113386-74-6]

$C_{10}H_{10}S_2$ M 194.321

Cunningham, D.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1021 (*uv*)

3,5-Dimethyl-2,3′-bithiophene, 9CI D-80433

[90655-30-4]

$C_{10}H_{10}S_2$ M 194.321
Bp_1 115-117°.

Gronowitz, S. *et al*, *Chem. Scr.*, 1983, **22**, 265 (*synth, pmr*)

4,4′-Dimethyl-2,2′-bithiophene, 9CI D-80434

[111372-97-5]

$C_{10}H_{10}S_2$ M 194.321
Mp 67°.

Cunningham, D.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1021 (*uv*)
Krische, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1476 (*synth, pmr*)

4,4′-Dimethyl-3,3′-bithiophene, 9CI D-80435

[15940-59-7]

$C_{10}H_{10}S_2$ M 194.321
Viscous oil. Bp_{10} 133-134°.

Gronowitz, S. *et al*, *Ark. Kemi*, 1967, **27**, 153 (*synth, pmr*)
Wiklund, E. *et al*, *Chem. Scr.*, 1973, **3**, 226 (*pmr*)

5,5′-Dimethyl-2,2′-bithiophene, 9CI D-80436

$C_{10}H_{10}S_2$ M 194.321
Shows nematocidal props. Cryst. (MeOH), plates (pentane). Mp 68° (64-65°).

Lescot, E. *et al*, *J. Chem. Soc.*, 1959, 3234 (*synth*)
Uhlenbroek, J.H. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1960, **79**, 1181 (*uv, pharmacol*)
Curtis, R.F. *et al*, *J. Chromatogr.*, 1962, **9**, 366 (*chromatog*)
Atkinson, R.E. *et al*, *J. Chem. Soc. C*, 1967, 2011 (*synth, ir, chromatog*)
Abu-Eittah, R.H. *et al*, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 2126 (*synth, uv*)
Krische, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1476 (*synth, pmr*)

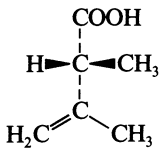
5,5′-Dimethyl-3,3′-bithiophene, 9CI D-80437

[38418-27-8]

$C_{10}H_{10}S_2$ M 194.321
Flakes (ligroin). Mp 135-136°.

Gronowitz, S. *et al*, *Acta Chem. Scand.*, 1962, **16**, 1127 (*synth, pmr*)
Norden, B. *et al*, *Acta Chem. Scand.*, 1972, **26**, 429 (*uv, conformn*)
Wiklund, E. *et al*, *Chem. Scr.*, 1973, **3**, 226 (*pmr*)

2,3-Dimethyl-3-butenoic acid D-80438



(*R*)-*form*

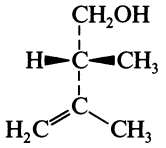
$C_6H_{10}O_2$ M 114.144

(R)-form

Liq. Bp_{42} 120°. $[\alpha]_D^{25}$ −27° (0.73 in $CHCl_3$) (71% e.e.).

Walba, D.M. *et al*, *J. Org. Chem.*, 1988, **55**, 1046 (*synth, ir, pmr, cmr, ms*)

2,3-Dimethyl-3-buten-1-ol D-80439



$C_6H_{12}O$ M 100.160

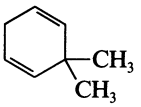
(R)-form

Liq. Bp_{78} 87°.

Walba, D.M. *et al*, *J. Org. Chem.*, 1988, **53**, 1046 (*synth, ir, pmr, cmr, ms*)

3,3-Dimethyl-1,4-cyclohexadiene D-80440

[35934-83-9]

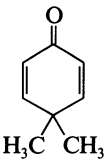


C_8H_{12} M 108.183
Liq. Bp 110-113° (91% pure) .

Stoos, F. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2719 (*synth*)
Jacobson, B.M. *et al*, *J. Org. Chem.*, 1988, **53**, 3247 (*synth*)

4,4-Dimethyl-2,5-cyclohexadien-1-one D-80441

[1073-14-9]

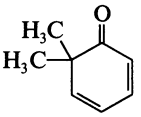


$C_8H_{10}O$ M 122.166
$Bp_{0.15}$ 41°.

Zimmerman, H.E. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 6589; 1971, **93**, 3653 (*synth*)

6,6-Dimethyl-2,4-cyclohexadien-1-one D-80442

[21428-63-7]

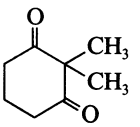


$C_8H_{10}O$ M 122.166
Liq. d_4^{20} 0.964. n_D^{20} 1.4992. Rearr. on htg. to phenols.

Alder, K. *et al*, *Chem. Ber.*, 1957, **90**, 1709.

2,2-Dimethyl-1,3-cyclohexanedione D-80443

[562-13-0]



$C_8H_{12}O_2$ M 140.182
Cryst. Mp 39-40°. Bp_{11} 103-105°.

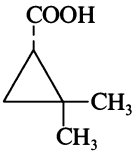
Dioxime:

$C_8H_{14}N_2O_4$ M 202.210
Cryst. (EtOH). Mp 195-195.5°.

Swaminathan, S. *et al*, *Tetrahedron*, 1964, **20**, 1119 (*synth, ir*)
Jacobson, B.M. *et al*, *J. Org. Chem.*, 1988, **53**, 3247 (*synth*)

2,2-Dimethylcyclopropanecarboxylic acid D-80444

[931-26-0]



(*S*)-*form*

$C_6H_{10}O_2$ M 114.144

(*S*)-*form* [14590-53-5]
Liq. $[\alpha]_D^{20}$ +132° (c, 1.01 in MeOH), $[\alpha]_D^{20}$ +142° (c, 1.01 in $CHCl_3$).

Amide:
$C_6H_{11}NO$ M 113.159
Mp 136-137.5°. $[\alpha]_D^{20}$ +101.4° (c, 1.0 in $CHCl_3$).

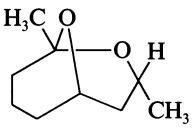
(±)-*form* [75885-59-5]
Liq. Bp 198-201°, Bp_5 83-84°.

Amide: Needles (EtOAc). Mp 177-177.5°.

Nitrile: 2-Cyano-1,1-dimethylcyclopropane
C_6H_9N M 95.144
Liq. $d_{20}^{24.6}$ 0.85. Bp 154.5-155.5°.

Nelson, E.R. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 3467 (*synth, deriv*)
Graham, D.W. *et al*, *J. Med. Chem.*, 1987, **30**, 1074 (*resoln, abs config, cryst struct, pmr*)

1,3-Dimethyl-2,9-dioxabicyclo-[3.3.1]nonane D-80445



$C_9H_{16}O_2$ M 156.224

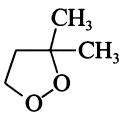
(*1R,3R*)-*form* [76740-34-6]
Isol. from Norway spruce infected with the ambrosia beetle *Trypodendron lineatum*. Host-specific pheromone. Liq. $[\alpha]_D^{24}$ −37.9° (c, 0.5 in pentane).

[63013-24-1, 63013-25-2, 76334-10-6, 76740-35-7, 76740-36-8]

Mori, Y. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1078 (*synth, pmr, bibl*)

3,3-Dimethyl-1,2-dioxolane D-80446

[67393-70-8]

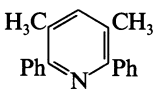


$C_5H_{10}O_2$ M 102.133
Bp_{16} 52-54°.

Nixon, J.R. *et al*, *J. Org. Chem.*, 1978, **43**, 4048 (*synth, pmr*)
Bloodworth, A.J. *et al*, *J. Org. Chem.*, 1986, **51**, 2110 (*synth, pmr, cmr*)

3,5-Dimethyl-2,6-diphenylpyridine, 9CI D-80447

[14435-89-3]



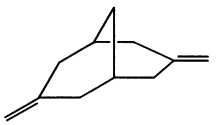
$C_{19}H_{17}N$ M 259.350
Cryst. solid (hexane/$CHCl_3$). Mp 136-137°.

Newkome, G.R. *et al*, *J. Org. Chem.*, 1972, **37**, 1329 (*synth, pmr, uv*)
Barluenga, J. *et al*, *J. Org. Chem.*, 1988, **53**, 5960 (*synth, pmr, cmr*)

2,6-Dimethylenebicyclo[3.3.1]nonane D-80448

2,6-Bis(methylene)bicyclo[3.3.1]nonane

[26069-13-6]



$C_{11}H_{16}$ M 148.247
Liq. Bp 185-190°, Bp_{15} 73-75°.

Landa, S. *et al*, *Collect. Czech. Chem. Commun.*, 1970, **35**, 1005 (*synth*)
Bishop, R. *et al*, *Aust. J. Chem.*, 1979, **32**, 2675 (*synth, ir, pmr, cmr*)

4,5-Dimethyl-2,3-furandicarboxylic acid D-80449

[111301-74-7]

$C_8H_8O_5$ M 184.148
Powder. Mp 243-244°.

Mann, J. *et al*, *Tetrahedron*, 1987, **43**, 2533 (*synth, ir*)

4,4-Dimethyl-6-heptenoic acid, 9CI D-80450

[92611-60-4]

$H_2C{=}CHCH_2C(CH_3)_2CH_2CH_2COOH$

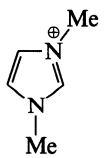
$C_9H_{16}O_2$ M 156.224
Oil. Bp_1 80-90°.

S-*Benzylisothiouronium salt:* [116914-27-3].
Cryst. (H_2O). Mp 140-141°.

Me ester: [113086-97-8].
$C_{10}H_{18}O_2$ M 170.251
Oil. Bp_{12} 78-82°.

Pattenden, G. *et al*, *Tetrahedron*, 1987, **43**, 5637 (*synth, ir, pmr, cmr*)

1,3-Dimethyl-1*H*-imidazolium(1+), 9CI D-80451



$C_5H_9N_2^{\oplus}$ M 97.139

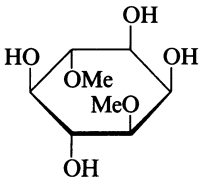
Iodide: [4333-62-4].
$C_5H_9IN_2$ M 224.044
Prisms (EtOAc). Mp 86.5-88°.

Picrate: Yellow cryst. (EtOH). Mp 100-103°.

Overberger, C.G. *et al*, *J. Org. Chem.*, 1965, **30**, 3580 (*synth*)
Karkhanis, D.W. *et al*, *Phosphorus Sulfur*, 1985, **22**, 49 (*synth*)
Org. Synth., 1986, **64**, 92 (*synth, pmr, cmr*)

1,4-Di-*O*-methyl-*myo*-inositol D-80452

Liriodendritol



(–)-*form*

$C_8H_{16}O_6$ M 208.211

(–)-***form*** [22006-88-8]

Isol. from *Liriodendron tulipifera*, *L. chinense* and other plants. Prisms (EtOH). Mp 224° (anhyd.). $[\alpha]_D$ –25° (H_2O).

Tetra-Ac:

$C_{16}H_{24}O_{10}$ M 376.360

Mp 139°. $[\alpha]_D$ –24° ($CHCl_3$).

(±)-***form***

Mp 203°.

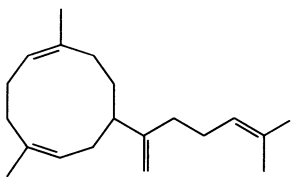
Tetra-Ac: Cryst. (EtOH aq.). Mp 155-156°.

Angyal, S.J. *et al*, *J. Chem. Soc.*, 1961, 4718 (*struct*, *synth*)
Kindl, H. *et al*, *Fortschr. Chem. Org. Naturst.*, 1966, **24**, 149 (*rev*)

1,5-Dimethyl-8-(5-methyl-1-methylene-4-hexenyl)-1,5-cyclodecadiene, 9CI D-80453

13-Prenyl-1(10),4,11-germacratriene

[122616-70-0]

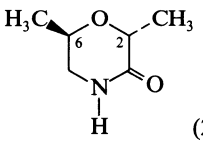


$C_{20}H_{32}$ M 272.473

Constit. of *Helichrysum argyrophyllum*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

2,6-Dimethyl-3-morpholinone D-80454



(2*R*,6*R*)-*form*

$C_6H_{11}NO_2$ M 129.158

(2*R*,6*R*)-***form*** [117465-49-3]

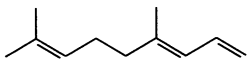
Cryst. (CH_2Cl_2/C_6H_6). Mp 83-85°. $[\alpha]_D^{20}$ –20.8° (c, 1.0 in $CHCl_3$). (2*R*,6*S*) and (2*S*,6*S*)-isomers also prepd., as a diastereoisomericmixt.

[117465-50-6, 117465-51-7, 117465-54-0]

Danklmaier, J. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 1149 (*synth*, *pmr*, *cmr*)

4,8-Dimethyl-1,3,7-nonatriene D-80455

Updated Entry replacing D-50644



$C_{11}H_{18}$ M 150.263

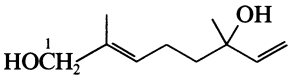
(*E*)-***form***

Constit. of essential oil of *Elettaria cardamomum*, *Rosa* spp., *Magnolia liliflora*. Oil.

[21214-62-0]

Pattenden, G. *et al*, *J. Chem. Soc. C*, 1968, 1984 (*synth*)
Maurer, B. *et al*, *Tetrahedron Lett.*, 1986, **27**, 2111 (*struct*, *synth*)
Boland, W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 247 (*biosynth*, *bibl*)

2,6-Dimethyl-2,7-octadiene-1,6-diol D-80456



(*E*)-*form*

$C_{10}H_{18}O_2$ M 170.251

(*E*)-***form***

9-*Hydroxylinalool*

1-O-β-D-Glucoside: [64776-96-1]. ***Betulalbuside*** **A**

$C_{16}H_{28}O_7$ M 332.393

Constit. of *Betula alba* and *Chaenomeles japonica*. Oil. 6-config not detd.

(*Z*)-***form***

1-*Hydroxylinalool*

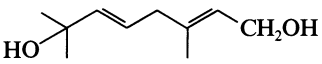
1-O-*β-D-Glucoside:* [64813-08-7]. ***Betulalbuside*** **B**

$C_{16}H_{28}O_7$ M 332.393

From *B. alba* and *C. japonica*. Oil. 6-config. not detd.

Tschesche, R. *et al*, *Chem. Ber.*, 1977, **110**, 3111.

3,7-Dimethyl-2,5-octadiene-1,7-diol D-80457



$C_{10}H_{18}O_2$ M 170.251

1-Ac: [33766-42-6]. *8-Acetoxy-2,6-dimethyl-3,6-octadien-2-ol*

$C_{12}H_{20}O_3$ M 212.288

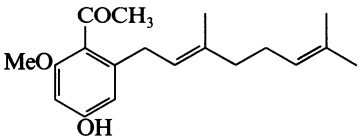
Constit. of *Jasonia montana*. Oil.

Ahmed, A.A. *et al*, *Phytochemistry*, 1988, **27**, 3875.

2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone D-80458

1-[2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyphenyl]ethanone, 9CI

[121379-44-0]



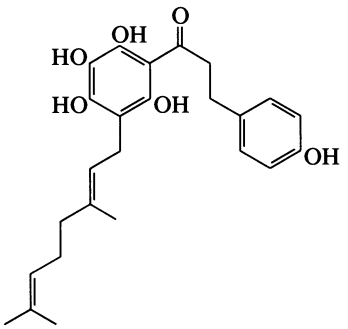
$C_{19}H_{26}O_3$ M 302.413

Constit. of *Dioscorea bulbifera*. Cryst. Mp 225°.

Gupta, D. *et al*, *Phytochemistry*, 1989, **28**, 947.

1-[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,5,6-tetrahydroxyphenyl]-3-(4-hydroxyphenyl)-1-propanone,9CI **D-80459**

2′,4,4′,5′,6-Pentahydroxy-3′-neryldihydrochalcone.
2′,4,4′,5′,6′-Pentahydroxy-3′-geranyldihydrochalcone



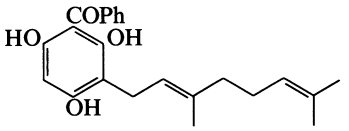
$C_{25}H_{30}O_6$ M 426.508
Isol. from *Helichrysum monticola*. Oil. Unseparated mixt. of (*E*)- and (*Z*)- forms.

[76015-50-4, 76015-51-5]

Bohlmann, F. *et al*, *Phytochemistry*, 1980, **19**, 683.

3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzophenone **D-80460**

[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-trihydroxyphenyl]phenylmethanone, 9CI. 3-Geranyl-2,4,6-trihydroxybenzophenone



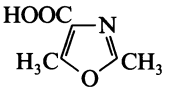
(*E*)-*form*

$C_{23}H_{26}O_4$ M 366.456
(***E***)-***form*** [70219-87-3]
2-*Benzoyl-6-geranylphloroglucinol*
Isol. from *Leontonyx* spp. and *Helichrysum* spp. Oil.
(***Z***)-***form*** [76015-48-0]
2-*Benzoyl-6-nerylphloroglucinol*
$C_{23}H_{26}O_4$ M 366.456
Isol. from *H. monticola*. Oil.

Bohlmann, F. *et al*, *Phytochemistry*, 1978, **17**, 1929; 1979, **18**, 2046; 1980, **19**, 683.

2,5-Dimethyl-4-oxazolecarboxylic acid, 9CI **D-80461**

[23000-14-8]

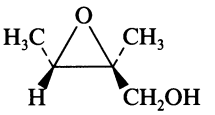


$C_6H_7NO_3$ M 141.126
Cryst. (MeOH). Mp 236-237° (220° dec.).
Et ester:
$C_8H_{11}NO_3$ M 169.180
Bp_{22} 125°, Bp_{11} 117°.
Amide:
$C_6H_8N_2O_2$ M 140.141
Cryst. (H_2O). Mp 234°.
Nitrile: 4-Cyano-2,5-dimethyloxazole
$C_6H_6N_2O$ M 122.126
Oil. Bp_{18} 84-85°.

Treibs, A. *et al*, *Chem. Ber.*, 1951, **84**, 96 (*synth, ester, amide*)
Brown, D.J. *et al*, *J. Chem. Soc. B*, 1969, 270 (*pmr*)
Doleschall, G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1875 (*synth, ir, pmr*)

2,3-Dimethyloxiranemethanol **D-80462**

2,3-Epoxy-2-methyl-1-butanol



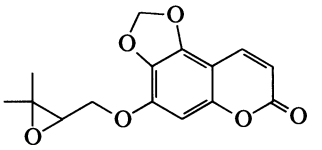
$C_5H_{10}O_2$ M 102.133
(***2S,3S***)-***form*** [113531-34-3]
Oil. Bp_5 120° (oven) . $[\alpha]_D$ −22.2° (c, 3.0 in CH_2Cl_2). 94% ee.

Evans, D.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2506 (*synth, ir, pmr, cmr*)

7-(3,3-Dimethyloxiranyl)methoxy-5,6-methylenedioxycoumarin **D-80463**

4-(3,3-Dimethyloxiranyl)methoxy-7H-1,3-dioxolo[4,5-f][1]benzopyran-7-one, 9CI

[57419-59-7]



$C_{15}H_{14}O_6$ M 290.272
Isol. from *Pteronia glabrata*. Mp 81°. $[\alpha]_D$ +22° ($CHCl_3$).

Bohlmann, F. *et al*, *Chem. Ber.*, 1975, **108**, 2955.

2,2-Dimethyl-4-oxo-1-pentanal **D-80464**

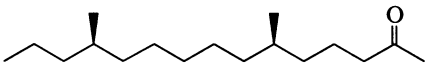
[61031-76-3]

$H_3CCOCH_2C(CH_3)_2CHO$

$C_7H_{12}O_2$ M 128.171
Bp_{20} 84-86°.

Magnus, P.D. *et al*, *Synth. Commun.*, 1980, **10**, 273 (*synth, ir, pmr*)
Hudlicky, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4735 (*synth, ir, pmr*)

6,12-Dimethyl-2-pentadecanone **D-80465**



(6*R*,12*R*)-*form*

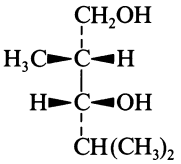
$C_{17}H_{34}O$ M 254.455
Sex pheromone of the banded cucumber beetle *Diabrotica balteata* (abs. config. of nat. pheromone not yet known).
(***6R,12R***)-***form***
$Bp_{0.29}$ 108-111°. $[\alpha]_D^{22}$ −0.5° (c, 1.13 in $CHCl_3$). n_D^{22} 1.4388.
(***6R,12S***)-***form***
$Bp_{0.29}$ 104-107°. $[\alpha]_D^{20}$ +1.9° (c, 1.16 in $CHCl_3$). n_D^{20} 1.4392.
(***6S,12R***)-***form***
$Bp_{0.28}$ 114-117°. $[\alpha]_D^{20}$ −1.9° (c, 1.14 in $CHCl_3$). $n_D^{19.5}$ 1.4392.
(***6S,12S***)-***form***

$Bp_{0.2}$ 108-113°. $[\alpha]_D^{21}$ +0.5° (c, 1.06 in $CHCl_3$). n_D^{21} 1.4393.

Mori, K. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 717 (*synth, pmr, cmr, abs config, bibl*)

2,4-Dimethyl-1,3-pentanediol D-80466

[60712-38-1]



(2*R*,3*R*)-*form*

$C_7H_{16}O_2$ M 132.202

(2R,3R)-form [82335-99-7]
Mp 84-85°. $[\alpha]_D$ −16.4° (c, 0.04 in $CHCl_3$).

(2S,3R)-form [97906-32-6]
Cryst. Mp 43-45°. $[\alpha]_D^{20}$ +16.5° (c, 1.1 in CH_2Cl_2). Not optically pure.

3-O-Benzoyl: [113778-42-0].
$C_{14}H_{20}O_3$ M 236.310
Oil. $Bp_{0.5}$ 115°.

(2S,3S)-form [98391-91-4]
$[\alpha]_D^{25}$ +11.3° (c, 0.6 in $CHCl_3$).

(2RS,3RS)-form [103729-84-6]
(±)-erythro-*form*
Prisms. Mp 53.0-54.5°. The *erythro* label is ambiguous.

[3876-47-9, 98391-91-4, 103729-88-0]

Wood, R.D. *et al*, *Tetrahedron Lett.*, 1982, **23**, 707 (*synth, pmr, ms*)
Helmchen, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 874 (*synth, abs config*)
Masamune, S. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 8279 (*synth*)
Evans, D.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3560 (*synth, ir, pmr, cmr*)
Baker, R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 85 (*synth, uv, pmr, ms*)

3,3-Dimethyl-4-pentynal, 9CI D-80467

[35849-64-0]

$HC{\equiv}CC(CH_3)_2CH_2CHO$

$C_7H_{10}O$ M 110.155
Liq. Bp 132-134°, Bp_{140} 75-80°.

Oxime:
$C_7H_{11}NO$ M 125.170
Bp_{42} 120-122°.

2,4-Dinitrophenylhydrazone: Cryst. (EtOH). Mp 100-101°.

Di-Me acetal: [82850-96-2]. *5,5-Dimethoxy-3,3-dimethyl-1-pentyne, 9CI*
$C_9H_{16}O_2$ M 156.224
Liq. Bp_{15} 75-80°.

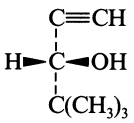
[34718-63-3, 35849-90-2]

Stevens, R.V. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 6629 (*synth, ir, pmr*)
McMurry, J.E. *et al*, *Tetrahedron*, 1987, **43**, 5489 (*synth, ir, pmr*)

4,4-Dimethyl-1-pentyn-3-ol, 9CI D-80468

tert-*Butylethynylcarbinol*

[19115-28-7]



R-form

$C_7H_{12}O$ M 112.171

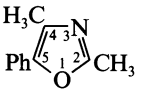
(R)-form [61317-72-4]
Liq. $[\alpha]_D^{20}$ +17.95° (neat).

(±)-form [61348-37-6]
Liq. Bp_{45} 75°.

Barrelle, M. *et al*, *Ann. Chim.* (*Paris*), 1967, **2**, 243 (*synth*)
Vigneson, J.-P. *et al*, *Tetrahedron Lett.*, 1979, 2683 (*synth*)
Henderson, M.A. *et al*, *J. Org. Chem.*, 1988, **53**, 4736 (*synth, ir, pmr, cmr, resoln*)

2,4-Dimethyl-5-phenyloxazole, 9CI D-80469

[23012-31-9]



$C_{11}H_{11}NO$ M 173.214
Mp 51-52°. Bp_{12} 129-131°, $Bp_{0.15}$ 75°.

Picrate: [56965-53-8].
Mp 170-172°.

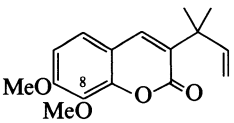
Bachstez, M., *Chem. Ber.*, 1914, **47**, 3163 (*synth*)
Bredereck, H. *et al*, *Chem. Ber.*, 1960, **93**, 1389 (*synth*)
Brown, D.J. *et al*, *J. Chem. Soc. B*, 1969, 270 (*pmr, props*)

3-(1,1-Dimethyl-2-propenyl)-7,8-dimethoxy-2*H*-1-benzopyran-2-one, 9CI D-80470

Updated Entry replacing D-10609

3-(1,1-Dimethylallyl)-7,8-dimethoxycoumarin

[30310-54-4]



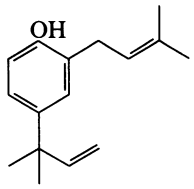
$C_{16}H_{18}O_4$ M 274.316
Isol. from roots of *Ruta graveolens*. Cryst. (hexane). Mp 85-86°.

8-O-De-Me: [61899-42-1]. ***3-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2H-1-benzopyran-2-one.*** *3-(1,1-Dimethylallyl)-8-hydroxy-7-methoxycoumarin*
$C_{15}H_{16}O_4$ M 260.289
Isol. from *R.* spp. Mp 98-100°.

Reisch, J. *et al*, *Tetrahedron Lett.*, 1970, 4305 (*isol*)
Gonzalez, A.G. *et al*, *An. Quim.*, 1976, **72**, 191 (*isol, synth, deriv*)

4-(1,1-Dimethyl-2-propenyl)-2-(3-methyl-2-butenyl)phenol D-80471

[73215-04-0]



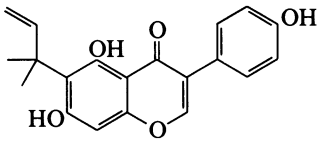
$C_{16}H_{22}O$ M 230.349
Constit. of *Perithalia caudata*. Oil.

Blackman, A.J. *et al*, *Aust. J. Chem.*, 1979, **32**, 2783.

6-(1,1-Dimethyl-2-propenyl)-4′,5,7-trihydroxyisoflavone D-80472

*6-(1,1-Dimethyl-2-propenyl)-5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*

[77390-42-2]



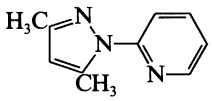
$C_{20}H_{18}O_5$ M 338.359
Incorr. reported as $C_{21}H_{18}O_5$. May be the 8-alkyl isomer. Isol. from wood of *Moghania macrophylla*. Prisms ($CHCl_3$/MeOH). Mp 123-124°.

Krishnamurty, H.G. *et al*, *Phytochemistry*, 1980, **19**, 2797 (*isol, ir, pmr, ms, struct*)

2-(3,5-Dimethyl-1*H*-pyrazol-1-yl)pyridine D-80473

N-*(2-Pyridinyl)-3,5-dimethylpyrazole*

[21018-71-3]



$C_{10}H_{11}N_3$ M 173.217
Bidentate ligand; extraction agent for Cd(II), Hg(II) and Pb(II). Light yellow oil. $Bp_{0.4}$ 74°.

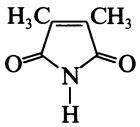
B,HCl: Mp 140-144°.

Saha, N. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1236 (*synth*)
Baker, A.T. *et al*, *Aust. J. Chem.*, 1989, **42**, 623 (*bibl*)

3,4-Dimethyl-1*H*-pyrrole-2,5-dione, 9CI D-80474

3,4-Dimethylmaleimide. 2,5-Dioxo-3,4-dimethyl-Δ^3-pyrroline

[17825-86-4]



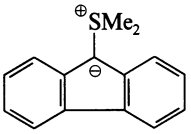
$C_6H_7NO_2$ M 125.127
Cryst. (EtOH). Mp 118-119°.

Dioxime: [14445-80-8].
$C_6H_9N_3O_2$ M 155.156
Cryst. (EtOH). Mp >300° dec.

Otto, R. *et al*, *Ber.*, 1885, **18**, 825 (*synth*)
Bischoff, C.A., *Ber.*, 1900, **33**, 1416 (*synth*)
Plieninger, H. *et al*, *Justus Liebigs Ann. Chem.*, 1968, **711**, 130 (*synth*)
Alonso Garrido, D.O. *et al*, *J. Org. Chem.*, 1988, **53**, 403 (*dioxime, synth, pmr*)

Dimethylsulfonium 9-fluorenylide D-80475

[72393-25-0]



$C_{15}H_{14}S$ M 226.342
Pale yellow solid. Mp 126-127° (70-75°). Unstable in air.

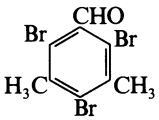
B,HBr: Hexagonal plates ($MeNO_2$). Mp 133°.

Picrate: Needles (H_2O). Mp 149-150°.

Ingold, C.K. *et al*, *J. Chem. Soc.*, 1930, 713 (*synth, props*)
Johnson, A.W. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 417 (*synth*)
Zhang, J.-J. *et al*, *J. Org. Chem.*, 1988, **53**, 716 (*synth, pmr, cmr*)

3,5-Dimethyl-2,4,6-tribromobenzaldehyde D-80476

[114634-34-3]

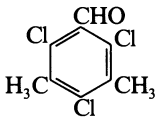


$C_9H_7Br_3O$ M 370.866
Cryst. Mp 224-225°.

Banfi, S. *et al*, *J. Org. Chem.*, 1988, **53**, 2863 (*synth, pmr*)

3,5-Dimethyl-2,4,6-trichlorobenzaldehyde D-80477

[114634-35-4]

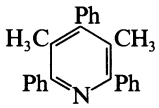


$C_9H_7Cl_3O$ M 237.512
Cryst. Mp 192-194°.

Banfi, S. *et al*, *J. Org. Chem.*, 1988, **53**, 2863 (*synth, pmr*)

3,5-Dimethyl-2,4,6-triphenylpyridine D-80478

[78018-66-3]

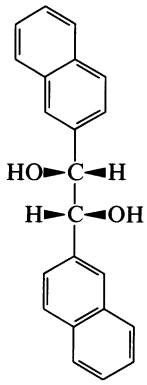


$C_{25}H_{21}N$ M 335.448
Cryst. solid (hexane/$CHCl_3$). Mp 154-156°.

Galiah, V. *et al*, *J. Indian Chem. Soc.*, 1955, **32**, 274 (*synth*)
Barluenga, J. *et al*, *J. Org. Chem.*, 1988, **53**, 5960 (*synth, ir, pmr, cmr*)

1,2-Di-2-naphthalenyl-1,2-ethanediol, 9CI D-80479

2-Hydronaphthoin



(1*R**,2*R**)-*form*

$C_{22}H_{18}O_2$ M 314.383

(1R*,2R*)-form [113469-20-8]

Cryst. + H_2O. Mp 237-238°. $[\alpha]_D^{23}$ +212° (c, 1.04 in THF). (−)-form also descr.

(1RS,2RS)-form [3408-28-4]

(±)-*form*

Cryst. + H_2O (C_6H_6). Mp 218-219°.

Di-Ac:

$C_{26}H_{22}O_4$ M 398.457

Cryst. (EtOAc). Mp 187-188°.

(1RS,2SR)-form

meso-*form*

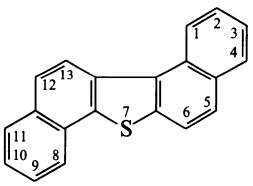
Plates (xylene), microcryst. (dioxan). Mp 261-262°.

Di-Ac: Cryst. (Py or xylene). Mp 205-207°.

Badger, G.M., *Nature (London)*, 1950, **165**, 647 (*synth*)
Mondodoev, G.T. *et al*, *J. Org. Chem. USSR (Engl. Transl.)*, 1965, **1**, 1257 (*synth*)
Chênevert, R. *et al*, *Synthesis*, 1987, 739 (*synth, resoln, ir, pmr*)

Dinaphtho[1,2-*b*:1′,2′-*d*]thiophene D-80480

[207-94-3]



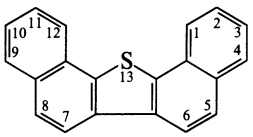
$C_{20}H_{12}S$ M 284.381

Leaflets. Mp 162°.

Tedjamulia, M.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1143 (*synth, pmr*)

Dinaphtho[1,2-*b*:2′,1′-*d*]thiophene D-80481

[239-72-5]



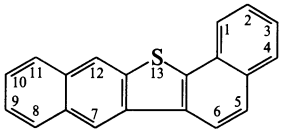
$C_{20}H_{12}S$ M 284.381

Cryst. ($CHCl_3$). Mp 255°.

Tedjamulia, M.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1143 (*synth, pmr*)
Klemm, L.H. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1111 (*synth, uv, pmr*)

Dinaphtho[1,2-*b*:2′,3′-*d*]thiophene D-80482

[239-94-1]



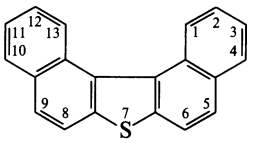
$C_{20}H_{12}S$ M 284.381

Beige solid ($CHCl_3$), pale yellow flakes. Mp 321°.

Tedjamulia, M.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1143 (*synth, pmr*)
Klemm, L.H. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1111 (*synth, uv, pmr*)
Johnston, M.D. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1593 (*pmr*)

Dinaphtho[2,1-*b*:1′,2′-*d*]thiophene D-80483

[194-65-0]



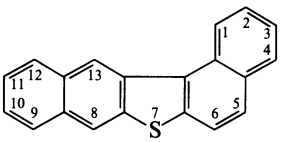
$C_{20}H_{12}S$ M 284.381

Cryst. Mp 206-207°.

Tedjamulia, M.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1143 (*synth, pmr*)

Dinaphtho[2,1-*b*:2′,3′-*d*]thiophene D-80484

[204-93-3]



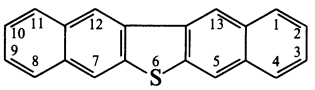
$C_{20}H_{12}S$ M 284.381

Pale yellow flakes. Mp 196° (189°).

Tedjamulia, M.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1143 (*synth, pmr*)

Dinaphtho[2,3-*b*:2′,3′-*d*]thiophene D-80485

[242-53-5]



$C_{20}H_{12}S$ M 284.381

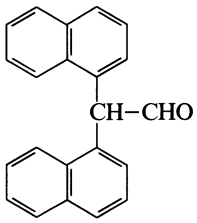
Fluorescent yellow leaves. Mp 265-266°.

Tedjamulia, M.L. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1143 (*synth, pmr*)

2,2-Di-(1-naphthyl)ethanal D-80486

α-1-Naphthalenyl-1-naphthaleneacetaldehyde, 9CI. 2,2-Di-(α-naphthyl)acetaldehyde

[98585-92-3]



$C_{22}H_{16}O$ M 296.368
Cream-coloured cryst. ($CHCl_3$). Mp 188-189°.

Zimmerman, H.E. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 7732 (*synth, ir, pmr, cmr*)

2,2-Di-(2-naphthyl)ethanal D-80487

α-2-Naphthalenyl-2-naphthaleneacetaldehyde. 2,2-Di-(β-naphthyl)acetaldehyde

[98586-00-6]

$C_{22}H_{16}$ M 280.368
Light yellow cryst. (CH_2Cl_2/hexane). Mp 163-164°.

Zimmerman, H.E. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 7732 (*synth, ir, pmr*)

2,2-Dinitroadamantane D-80488

Updated Entry replacing D-50699

2,2-Dinitrotricyclo[3.3.1.1^{3,7}]decane, 9CI

[88381-75-3]

$C_{10}H_{14}N_2O_4$ M 226.232
Cryst. (hexane). Mp 212-213°.

George, C. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 1674 (*cryst struct*)
Archibald, T.G. *et al*, *J. Org. Chem.*, 1988, **53**, 4645 (*synth, ir, pmr*)

2,4-Dinitroadamantane D-80489

2,4-Dinitrotricyclo[3.3.1.1^{3,7}]decane

$C_{10}H_{14}N_2O_4$ M 226.232
Cryst. (EtOH). Mp 175-180°.

Archibald, T.G. *et al*, *J. Org. Chem.*, 1988, **53**, 4645 (*synth, ir, pmr*)

2,6-Dinitroadamantane D-80490

2,6-Dinitrotricyclo[3.3.1.1^{3,7}]decane

$C_{10}H_{14}N_2O_4$ M 226.232
Cryst. (EtOH). Mp 165-170°.

Archibald, T.G. *et al*, *J. Org. Chem.*, 1988, **53**, 4645 (*synth, ir, pmr*)

4,6-Dinitro-1,3-benzenediol, 9CI D-80491

Updated Entry replacing D-70450

4,6-Dinitroresorcinol, 8CI

[616-74-0]

$C_6H_4N_2O_6$ M 200.107
Pale-yellow cryst. Mp 215°. pK_a 3.98.

▷ Synthesis produces explosive byprods.

Di-Ac:
$C_{10}H_8N_2O_8$ M 284.182
Mp 139°.

Me ether: [51652-35-8]. *5-Methoxy-2,4-dinitrophenol*
$C_7H_6N_2O_6$ M 214.134
Mp 113°.

Et ether: 5-Ethoxy-2,4-dinitrophenol
$C_8H_8N_2O_6$ M 228.161
Mp 77°.

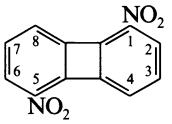
Di-Me ether: [1210-96-4]. *1,5-Dimethoxy-2,4-dinitrobenzene, 9CI, 8CI*
$C_8H_8N_2O_6$ M 228.161
Mp 157° (154°).

Di-Et ether: 1,5-Diethoxy-2,4-dinitrobenzene
$C_{10}H_{12}N_2O_6$ M 256.215
Mp 133°.

Pantlischenko, M. *et al*, *Monatsh. Chem.*, 1950, **81**, 293 (*synth*)
Rauner, W. *et al*, *Z. Chem.*, 1968, **8**, 338 (*synth*)
Granzhan, V.A. *et al*, *Zh. Strukt. Khim.*, 1971, **12**, 809; *CA*, **76**, 24579 (*ir*)
Crampton, M.R. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1972, 1178 (*deriv*)
Schmitt, R.J. *et al*, *J. Org. Chem.*, 1988, **53**, 5568 (*synth*)

1,5-Dinitrobiphenylene D-80492

[17532-86-4]



$C_{12}H_6N_2O_4$ M 242.190
Yellow needles (Me_2CO). Mp 272-274°.

Iqbal, K. *et al*, *J. Chem. Soc. C*, 1967, 1690 (*synth*)

2,6-Dinitrobiphenylene D-80493

$C_{12}H_6N_2O_4$ M 242.190
Deep yellow needles (EtOH). Subl. > 260°.

Baker, W. *et al*, *J. Chem. Soc.*, 1958, 2658, 2666 (*synth, uv*)

1,2-Dinitrocyclopropane D-80494

$C_3H_4N_2O_4$ M 132.076
(1RS,2RS)-form [109744-96-9]
(±)-trans-*form*
Cryst. (CCl_4). Mp 60-61°.

Wade, P.A. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 5452 (*synth, ir, pmr, cryst struct*)

1,12-Dinitrododecane D-80495

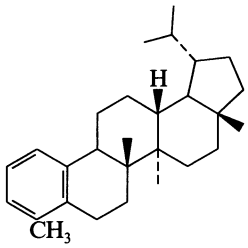
[110843-41-9]

$O_2NCH_2(CH_2)_{10}CH_2NO_2$

$C_{12}H_{24}N_2O_4$ M 260.333
Cryst. (MeOH). Mp 59-60°.

Ainscow, T.A. *et al*, *Tetrahedron*, 1987, **43**, 115 (*synth, ir, pmr*)

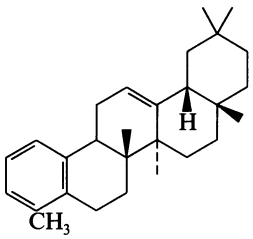
24,25-Dinor-1,3,5(10)-lupatriene D-80496



$C_{28}H_{42}$ M 378.640
Constit. of sediments.

Wolff, G.A. *et al*, *Tetrahedron*, 1989, **45**, 6721 (*synth*)

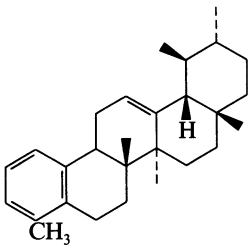
24,25-Dinor-1,3,5(10),12-oleanatetraene D-80497



$C_{28}H_{40}$ M 376.624
Constit. of sediments.

Wolff, G.A. *et al*, *Tetrahedron*, 1989, **45**, 6721 (*synth*)

24,25-Dinor-1,3,5(10),12-ursatetraene D-80498



$C_{28}H_{40}$ M 376.624
Constit. of sediments.

Wolff, G.A. *et al*, *Tetrahedron*, 1989, **45**, 6721 (*synth*)

4,9-Dioxa-1,6,11-dodecatriyne D-80499

1,4-Bis(2-propynyloxy)-2-butyne, 9CI

[83469-21-0]

$$HC{\equiv}CCH_2OCH_2C{\equiv}CCH_2OCH_2C{\equiv}CH$$

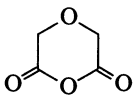
$C_{10}H_{10}O_2$ M 162.188
Oil. $Bp_{1.0}$ 78-81°.

Grigg, R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1357 (*synth, pmr, ir, ms*)

1,4-Dioxane-2,6-dione, 9CI D-80500

Diglycollic anhydride

[4480-83-5]

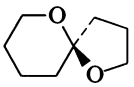


$C_4H_4O_4$ M 116.073
Cryst. (C_6H_6). Mp 91-93°. Bp_{12} 120°.

Anschutz, R., *Justus Liebigs Ann. Chem.*, 1890, **259**, 190 (*synth*)
Hurd, C.D. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 3490 (*synth*)
Brisse, F. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 2829 (*cryst struct*)

1,6-Dioxaspiro[4,5]decane D-80501

[177-23-1]



(R)-form

$C_8H_{14}O_2$ M 142.197

(R)-form [112996-24-4]
Oil. Bp_{30} 110-120° (bath) . $[\alpha]_D^{25}$ −44.4° (c, 0.635 in pentane).

(S)-form [112996-25-5]
Bp_{30} 110-120°. $[\alpha]_D$ +43.9° (c, 0.76 in pentane).

(±)-form
Oil.

Ley, S.V. *et al*, *Tetrahedron*, 1985, **41**, 3825 (*synth*)
Iwata, C. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4785 (*synth*)

1,3,2-Dioxathiane, 9CI D-80502

$C_3H_6O_2S$ M 106.145

2-Oxide: [4176-55-0]. *Trimethylene sulfite*
$C_3H_6O_3S$ M 122.145
d_4^{25} 1.33. Bp_{14} 66-67°.

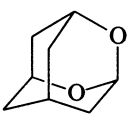
2,2-Dioxide: [1073-05-8]. *Trimethylene sulfate*
$C_3H_6O_4S$ M 138.144
Mp 60°.

de la Mare, P.B.D. *et al*, *J. Chem. Soc.*, 1956, 1813 (*synth, ir*)
Kaiser, E.T. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 602 (*oxides, synth, ir*)
Van Woerden, H.F. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1967, **86**, 353 (*oxide, synth*)
Lowe, G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1983, 1392 (*synth, pmr*)
Lowe, G. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 8512 (*dioxide, cryst struct*)

2,4-Dioxatricyclo[3.3.1.1^{3,7}]decane, 9CI D-80503

2,4-Dioxaadamantane

[13288-29-4]

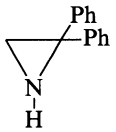


$C_8H_{12}O_2$ M 140.182
Cryst. (pentane or by subl.). Mp 210-212° (softens at 204°).

Briggs, A.J. *et al*, *Synthesis*, 1988, 66 (*synth, ms, ir, pmr*)

2,2-Diphenylaziridine D-80504

[25564-63-0]



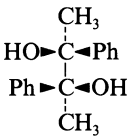
$C_{14}H_{13}N$ M 195.263
Oil. $Bp_{0.17}$ 111-115°.

Hahn, C.S. *et al*, *CA*, 1970, **72**, 78779s (*synth*)
Hassner, A. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 3733 (*synth, pmr*)
Perlman, M.E. *et al*, *J. Org. Chem.*, 1988, **53**, 1761 (*synth, ir, pmr*)

2,3-Diphenyl-2,3-butanediol, 9CI D-80505

Acetophenonepinacol

[1636-34-6]



(2*R*,3*R*)-*form*

$C_{16}H_{18}O_2$ M 242.317

(2R,3R)-form [33603-65-5]
$[\alpha]_D^{22}$ +31.4° (c, 0.5 in Et_2O).

(2S,3S)-form [63902-56-7]
Cryst. (EtOH). Mp 104.5-105°. $[\alpha]_D^{25}$ −34.4° (c, 2.7 in EtOH).

Di-Me ether: 2,3-Dimethoxy-2,3-diphenylbutane
$C_{18}H_{22}O_2$ M 270.371
Fine needles. Mp 93-94°. $[\alpha]_D^{24}$ +71.6° (c, 3.1 in $CHCl_3$).

(2RS,3RS)-form [22985-90-6]
(±)-*form*
Mp 125-126° (122-124°).

Di-Me ether: Mp 111-111.5°.

(2RS,3SR)-form [4217-65-6]
meso-*form*
Cryst. (EtOH). Mp 120°.

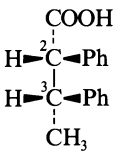
Di-Me ether: Cubes. Mp 171-173° (164-166°).

Cram, D.J. *et al*, *J. Am. Chem. Soc.*, 1959, 2748 (*synth, config, ir, deriv*)
Stocker, J.H. *et al*, *J. Am. Chem. Soc.*, 1960, 3913 (*synth*)
Stocker, J.H. *et al*, *J. Org. Chem.*, 1968, **33**, 294 (*synth*)
Seebach, D. *et al*, *Chem. Ber.*, 1977, **110**, 2316 (*synth*)
Reichel, L.W. *et al*, *Can. J. Chem.*, 1984, **62**, 424 (*synth*)
Nakayama, J. *et al*, *Tetrahedron Lett.*, 1987, **28**, 1799 (*synth, pmr, cmr*)

2,3-Diphenylbutanoic acid D-80506

Updated Entry replacing D-07796

β-Methyl-α-phenylbenzenepropanoic acid, 9CI. β-Methyl-α-phenylhydrocinnamic acid



(2*S*,3*R*)-*form*
Absolute configuration

$C_{16}H_{16}O_2$ M 240.301

(2S,3R)-form [52195-02-5]
(+)-erythro-*form*
Cryst. (Et_2O/pet. ether). Mp 185-186°. $[\alpha]_D^{26}$ +25.5° (c, 4 in EtOH).

(2RS,3SR)-form [33398-55-9]
(±)-erythro-*form*
Needles (EtOH). Mp 187-189°.

Amide: [16213-71-1].
$C_{16}H_{17}NO$ M 239.316
Cryst. Mp 193°.

Nitrile:
$C_{16}H_{15}N$ M 221.301
Bp_{13} 188-192°.

(2RS,3RS)-form [5350-86-7]
(±)-threo-*form*
Cryst. Mp 125-130° (133-134°).

Amide: [16213-72-2].
Cryst. Mp 173-174°.

Nitrile: [15645-55-3].
Needles. Mp 35-36°. Bp_{16} 210-212°.

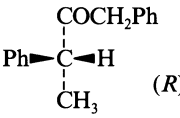
[5558-38-3, 52195-01-4, 56648-88-5]

Plentl, A.A. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 989 (*synth, derivs*)
Chambers, W.J. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 875 (*abs config*)
Auerbach, R.A. *et al*, *Tetrahedron*, 1971, **27**, 2069 (*synth, pmr*)
Ochiai, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 2525 (*synth*)

1,3-Diphenyl-2-butanone D-80507

Updated Entry replacing D-10653

[13363-25-2]



(*R*)-*form*

$C_{16}H_{16}O$ M 224.302

(R)-form [67504-36-3]
$[\alpha]_D$ −12.0° (c, 4.3 in C_6H_6, 41% ee).

(S)-form [59983-38-9]
$[\alpha]_D^{20}$ +88° (c, 1.0 in C_6H_6).

(±)-form
Bp_{40} 205-206°, Bp_2 138-139°.

Oxime:
$C_{16}H_{17}NO$ M 239.316
Mp 82-83°.

Semicarbazone: Mp 143-145°.

Levy, J. *et al*, *Bull. Soc. Chim. Fr.*, 1929, **45**, 94 (*synth*)
Perez-Ossorio, R. *et al*, *CA*, 1966, **65**, 19985 (*synth*)
Posner, G. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 3076 (*synth*)
Thompson, H.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 636 (*synth*)
Enders, D. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1976, **15**, 549 (*synth*)
Meyers, A.I. *et al*, *J. Org. Chem.*, 1978, **43**, 3245 (*abs config*)

2,4-Diphenyl-3-butyn-1-ol D-80508

[86100-15-4]

$PhC{\equiv}CCHPhCH_2OH$

$C_{16}H_{14}O$ M 222.286

(±)-form
Oil, cryst. on standing. Mp 51°.

Krause, N. *et al*, *Chem. Ber.*, 1988, **121**, 1315 (*synth, ir, pmr, ms*)

1,2-Diphenyl-1,2-cyclopropanedicarboxylic acid, 9CI D-80509

(1*RS*,2*RS*)-*form*

$C_{17}H_{14}O_4$ M 282.295

(1RS,2RS)-form [896-59-3]
(±)-trans-*form*
Cryst. (EtOH aq.). Mp 273°.

Di-Me ester: [111977-16-3].
$C_{19}H_{18}O_4$ M 310.349
Cryst. (EtOH). Mp 141-143°.

(1RS,2SR)-form [736-88-9]
cis-*form*
Cryst. (H_2O). Mp 175°.

Di-Me ester: [17160-34-8].
Cryst. (EtOH). Mp 138°.

Di-Et ester:
$C_{21}H_{22}O_4$ M 338.402
Cryst. (EtOH). Mp 76°.

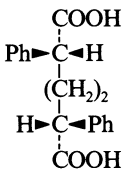
Anhydride:
$C_{17}H_{12}O_3$ M 264.280
Cryst. Mp 186°.

Bonavent, G. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 2462 (*synth, anhydride*)
Broser, W. *et al*, *Chem. Ber.*, 1967, **100**, 3472 (*synth*)
Hill, R.K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 497 (*synth, pmr*)

2,5-Diphenylhexanedioic acid D-80510

2,5-Diphenyladipic acid

[6622-43-1]



(2*RS*,5*RS*)-*form*

$C_{18}H_{18}O_4$ M 298.338

(2RS,5RS)-form
Mp 208°.

Dinitrile:
$C_{18}H_{16}N_2$ M 260.338
Cryst. (Et_2O). Mp 103-105°. Isomerises to *meso*-form on boiling in EtOH.

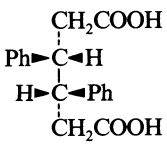
(2RS,5SR)-form [4070-63-7]
meso-*form*
Cryst. (AcOH). Mp 255-260° (266-267°).

Dinitrile: Cryst. (EtOH). Mp 173-175°.

Frank, C.E. *et al*, *Tetrahedron*, 1961, **26**, 303, 307 (*synth*)
U.S. Pat., 3 351 646, (1967); *CA*, **68**, 49723f (*synth*)
Casini, G. *et al*, *Tetrahedron*, 1972, **28**, 1497 (*synth, deriv*)

3,4-Diphenylhexanedioic acid, 9CI D-80511

3,4-Diphenyladipic acid



(3*R*,4*R*)-*form*

$C_{18}H_{18}O_4$ M 298.338

(3R,4R)-form [108391-57-7]
Cryst. (EtOH/AcOH). Mp 200-201°. $[\alpha]_D^{22}$ +13.1° (EtOH).

Dinitrile:
$C_{18}H_{16}N_2$ M 260.338
Mp 125-126°. $[\alpha]_D^{22}$ +20.3° ($CHCl_3$).

(3S,4S)-form [108391-56-6]
Mp 198-199°. $[\alpha]_D^{22}$ −11.0° (EtOH).

(3RS,4RS)-form [65610-00-6]
Mp 187°.

(3RS,4SR)-form [65610-01-7]
Needles (EtOH). Mp 270-271° (264-266°).

Dichloride:
$C_{18}H_{16}Cl_2O_2$ M 335.229
Cryst. (C_6H_6). Mp 187°.

[25347-44-8]

Oomen, M.P. *et al*, *J. Chem. Soc.*, 1930, 2148 (*synth*)
Shitov, G.G. *et al*, *Zh. Org. Khim.*, 1977, **13**, 2146; *CA*, **88**, 89229u (*synth*)
Toki, S. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1984, **1**, 152; *CA*, **100**, 191505 (*synth*)
Naemura, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 1675 (*synth, abs config, deriv synth*)

Diphenylketazine D-80512

Diphenylmethanone (diphenylmethylene)hydrazone, 9CI. Benzophenone azine. Bisdiphenylazimethylene

[983-79-9]

$$Ph_2C{=}N{-}N{=}CPh_2$$

$C_{26}H_{20}N_2$ M 360.457
Bright yellow cryst. solid (EtOH). Mp 162°.

Curtius, T. *et al*, *J. Prakt. Chem.*, 1891, **44**, 192 (*synth*)
Morton, A.A. *et al*, *J. Am. Chem. Soc.*, 1931, **53**, 2769 (*synth*)

5,5-Diphenyl-4-pentenoic acid, 9CI, 8CI D-80513

Updated Entry replacing D-08032

[5747-00-2]

$$Ph_2C{=}CHCH_2CH_2COOH$$

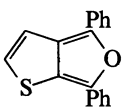
$C_{17}H_{16}O_2$ M 252.312
Cryst. Mp 82-83° (77-79°).

Me ester:
$C_{18}H_{18}O_2$ M 266.339
Mp 120°.

Fecht, H., *Ber.*, 1908, **41**, 2983 (*synth*)
Osman, A.M., *J. Prakt. Chem.*, 1969, **311**, 266 (*synth, pmr*)
Lehmann, J. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 827 (*synth, pmr*)

4,6-Diphenylthieno[2,3-*c*]furan D-80514

[105480-49-7]



$C_{18}H_{12}O_2S$ M 292.358
Fine yellow needles. Mp 139°.

Schöning, A. *et al*, *Chem. Ber.*, 1989, **122**, 1119 (*synth, uv, cmr, ms, cryst struct*)

Di-2-propenyl tetrasulfide, 9CI D-80515

Allyl tetrasulfide, 8CI. Diallyl tetrasulfide

[2444-49-7]

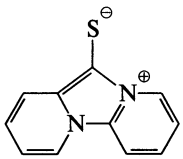
$$H_2C{=}CHCH_2{-}S{-}S{-}S{-}S{-}CH_2CH{=}CH_2$$

$C_6H_{10}S_4$ M 210.409
Isol. from garlic oil (*Allium sativum*) and from flowers and leaves of *Adenocalymna alliacea*. Oil with penetrating odour. Bp_{16} 122°.

Milligan, B. *et al*, *J. Chem. Soc.*, 1963, 3608 (*synth*)
Martin, D.J. *et al*, *Anal. Chem.*, 1966, **38**, 1604 (*pmr*)
Apparao, M. *et al*, *Phytochemistry*, 1978, **17**, 1660 (*isol*)
Block, E. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 7813 (*ms, cmr*)

Dipyrido[1,2-*a*: 1′,2′-*c*]imidazolium-11-thiolate D-80516

*11-Mercaptodipyrido[1,2-*a*: 1′,2′-*c*]imidazol-5-ium hydroxide, inner salt, 9CI*
[98779-37-4]

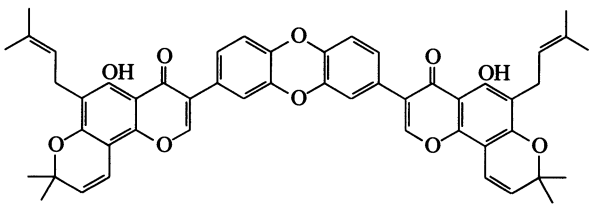


$C_{11}H_8N_2S$ M 200.264
Lustrous, dark maroon needles (EtOH). Mp 265-267° (under N_2), Mp 260-263° dec. (in air). Unstable to light.
B, HPF_6: Orange-yellow cryst. Mp 221-225° (under N_2).
B, $HClO_4$: [98779-74-9].
Cryst. Mp 237-239° (under N_2).
B,HBF_4: [98779-75-0].
Mp 216-217.5° (under N_2).
B,HI: [98779-76-1].
Mp 215.5-218° (under N_2).

Edward, J.T. *et al*, *J. Org. Chem.*, 1985, **50**, 4855 (*synth, ms*)

Disain D-80517

3,3′-Dibenzo[b,e][*1,4*]*dioxin-2,8-diylbis*[*5-hydroxy-8,8-dimethyl-6-(3-methyl-2-butenyl)-4*H,*8*H-*benzo*[*1,2*-b:*3,4*-b′]*dipyran-4-one*], *9CI*
[53755-80-9]

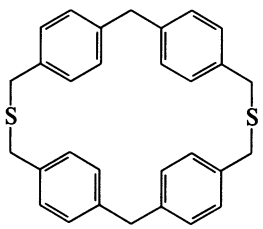


$C_{50}H_{44}O_{10}$ M 804.892
Isol. from *Maclura aurantiaca*. Oxidn. prod. of Osajin.

Nikonov, G.K. *et al*, *CA*, 1975, **82**, 13975q (*struct*)

2,18-Dithia[3.1.3.1]paracyclophane D-80518

8,20-Dithiapentacyclo[*20.2.2.2*^{3,6}*.2*^{10,13}*.2*^{15,18}]*dotriaconta-3,5,10,12,15,17,22,24,25,27,29,31-dodecaene, 9CI*
[114067-21-9]

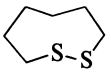


$C_{30}H_{28}S_2$ M 452.683
Needles (CH_2Cl_2).

Grützmacher, H.-F. *et al*, *Tetrahedron*, 1987, **43**, 3205 (*synth, pmr, ir, ms*)

1,2-Dithiocane D-80519

Updated Entry replacing D-50815
Hexamethylene disulfide. 1,2-Dithiacyclooctane
[6008-69-1]



$C_6H_{12}S_2$ M 148.293
Bp_2 65.5°. Readily polym.

Schoberl, A. *et al*, *Justus Liebigs Ann. Chem.*, 1958, **614**, 66 (*synth*)
Cragg, R.H. *et al*, *Tetrahedron Lett.*, 1973, 655 (*synth*)
Harpp, D.N. *et al*, *Tetrahedron Lett.*, 1986, **27**, 441 (*synth*)

2,3-Dodecadien-1-ol D-80520

[34656-66-1]

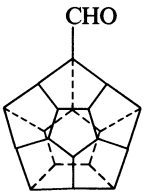
$$H_3C(CH_2)_7CH{=}C{=}CHCH_2OH$$

$C_{12}H_{22}O$ M 182.305

Landor, P.D. *et al*, 1971, 1638 (*synth, ir*)
Djahanbini, D. *et al*, *Tetrahedron*, 1987, **43**, 3441 (*synth, ir, pmr*)

Dodecahedranecarboxaldehyde D-80521

Tetradecahydro-5,2,1,6,3,4-[*2,3*]*butanediyl*[*1,4*]*diylidenedipentaleno*[*2,1,6*-cde:*2′,1′,6′*-gha]*pentalene-1*(2H)*-carboxaldehyde, 9CI. Formyldodecahedrane*
[112896-33-0]



$C_{21}H_{20}O$ M 288.388
Solid. Mp >250°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1303 (*synth, cmr*)

Dodecahedranecarboxylic acid D-80522

[112896-30-7]
$C_{21}H_{20}O_2$ M 304.388
Cryst. Mp >250°.

Me ester: [112896-31-8].
$C_{22}H_{22}O_2$ M 318.415
Solid. Mp 192-193°.

Amide: [112896-34-1].
$C_{21}H_{21}NO$ M 303.403
Solid. Mp >250°.

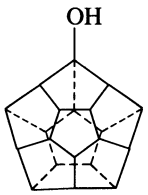
Nitrile: [116635-01-9]. *Cyanododecahedrane*
$C_{21}H_{19}N$ M 285.388
Solid. Mp >250°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1303 (*synth, cmr, ms*)
Weber, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5315 (*deriv, synth*)
Gallucci, J.C. *et al*, *Acta Crystallogr., Sect. C*, 1989, **45**, 893 (*cryst struct, ester*)

Dodecahedranol D-80523

*Tetradecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalen-1(2*H*)-ol, 9CI. Hydroxydodecahedrane*

[112896-36-3]



$C_{20}H_{20}O$ M 276.377
Solid. Mp >250°.

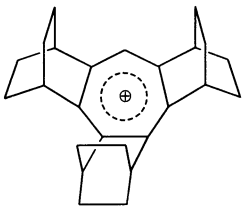
Trifluoroacetyl: [112925-47-0].
$C_{22}H_{19}F_3O_2$ M 372.386
Solid. Mp 183-185°.

O-*Nitrate:* [112896-38-5].
$C_{20}H_{19}NO_3$ M 321.375
Solid. Mp 220°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1303 (*synth, cmr*)

2,3,4,5,6,7,8,10,11,12,13,?-Dodecahydro-1,4:5,8:10,13-triethano-1*H*-tribenzo[*a,c,e*]cycloheptenylium(1+), 9CI D-80524

1,2:3,4:5,6-Tris(bicyclo[2.2.2]octeno)tropylium



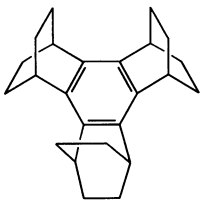
$C_{25}H_{31}^{\oplus}$ M 331.520
Thermodynamically very stable carbocation.

Hexafluoroantimonate: [112440-02-5].
$C_{25}H_{31}Cl_6Sb$ M 665.986
Mp 290-292° dec.

Komatsu, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 633 (*synth, uv, pmr, cmr*)

1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydro-1,4:5,8:9,12-triethanotriphenylene, 9CI D-80525

[112439-96-0]

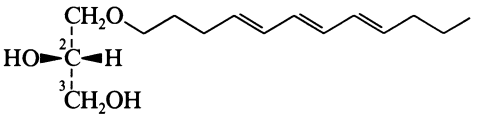


$C_{24}H_{30}$ M 318.501
Cryst. Mp 277-279°.

Komatsu, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 633 (*synth, uv, pmr, cmr*)

1-*O*-(4,6,8-Dodecatrienyl)glycerol D-80526

3-(4,6,8-Dodecatrienyloxy)-1,2-propanediol



$C_{15}H_{26}O_3$ M 254.369
Closely related to the fecapentaenes.

(S, all-E)-form

*2-*O*-(4-Hydroxybenzoyl):* ***Bretonin A***
$C_{22}H_{30}O_5$ M 374.476
Isol. from an unidentified marine demosponge. Oil. Opt. rotn. too small to measure.

*2-*O*-(4-Hydroxybenzoyl), di-Ac:* $[\alpha]_D^{25}$ −7.0° (c, 0.13 in $CHCl_3$).

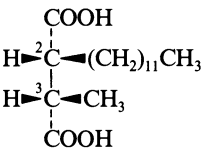
*3-*O*-(4-Hydroxybenzoyl):* ***Isobretonin A***
$C_{22}H_{30}O_5$ M 374.476
Isol. from an unidentified marine demosponge. Oil. $[\alpha]_D^{25}$ +7.3° ($CHCl_3$). Has (*R*-) config.

Guella, G. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1121 (*isol, uv, pmr, cmr, struct*)

2-Dodecyl-3-methylbutanedioic acid, 9CI D-80527

Updated Entry replacing C-00305

2-Dodecyl-3-methylsuccinic acid



$C_{17}H_{32}O_4$ M 300.437

(2R,3S)-form [22139-54-4] ***Roccellic acid***
Occurs in *Lecanora* spp., *Roccella tinctoria, Lepraria latebrarum, Lecidea aglaeotara, Pannaria languinosa* and other lichens. Cryst. (pet. ether). Mp 131-132°. $[\alpha]_D$ +17.4° (EtOH).

Di-Me ester: Cryst. (Et_2O). Mp 28-29°.

Phenylimide: Cryst. (MeOH). Mp 57-58°.

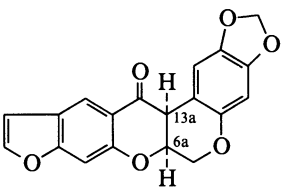
Åkermark, B., *Acta Chem. Scand.*, 1962, **16**, 599 (*abs config*)
Huneck, S. *et al*, *Phytochemistry*, 1969, **8**, 1301 (*isol*)
Huneck, S. *et al*, *Z. Naturforsch., B*, 1969, **24**, 750 (*isol*)
Åkermark, B., *Acta Chem. Scand.*, 1970, **24**, 1456 (*isol*)
Ollis, W.D. *et al*, *J. Chem. Soc. C*, 1971, 1318 (*isol*)

Dolineone D-80528

Updated Entry replacing D-08628

Dolichone

[10065-28-8]



$C_{19}H_{12}O_6$ M 336.300
CA numbering shown. Isol. from roots of *Neorautanenia pseudopachyrrhiza*, also from *Pachyrrhizus erosus*. Needles (MeOH). Mp 233-235°. $[\alpha]_D^{20}$ +135° (c, 1.3 in $CHCl_3$).

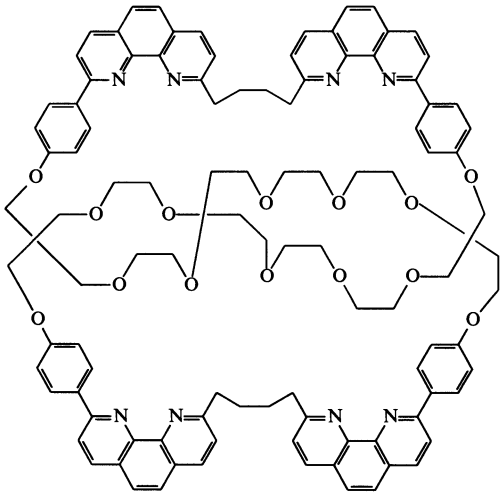
6a,13a-Didehydro: [28570-72-1]. ***Dehydrodolineone***
$C_{19}H_{10}O_6$ M 334.284

Isol. from *Neorautanenia amboensis* roots. Yellow needles. Mp 290-292°. Poss. artifact.

Crombie, L. *et al*, *J. Chem. Soc.*, 1963, 1569 (*isol*, *struct*)
Oberholzer, M.E. *et al*, *Tetrahedron Lett.*, 1974, 2211 (*Dehydrodolineone*)

7,8,9,10,24,25,27,28,30,31,33,34,36,37,39,40,54,55,56,57,71,72,74,75,77,78,80,1,83,84,86,87-Dotriacontahydro-1,93:4,6:11,13:16,18:19,22:42,45:46,48:51,53:58,60:63,65:66,69:89,92-dodecathenotetrabenzo[*z*,j_1,q_2,a_3][1,4,7,10,13,16,19,44,47,50,53,56,59,62,25,28,35,38,68,71,78,81]tetradecaoxaotaazacyclohexaoctacontine **D-80529**

[118798-04-2]

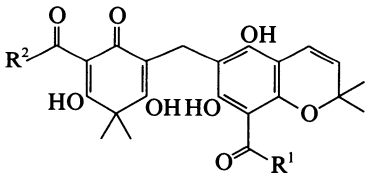


$C_{104}H_{104}N_8O_{14}$ M 1690.011
First molecule with trefoil knot topology. Glass.

Dietrich-Buchecker, C.O. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1989, **28**, 189.

Drummondin A **D-80530**

[119171-76-5]



$R^1 = R^2 = CH_2CH_3$

$C_{26}H_{30}O_8$ M 470.518
Constit. of *Hypericum drummondii*. Antimicrobial and cytotoxic agent. Yellow cryst. (hexane). Mp 130-132°.

Jayasuriya, H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 325 (*isol*, *pmr*, *cmr*)

Drummondin B **D-80531**

[119171-77-6]

As Drummondin A, D-80530 with

$R^1 = CH_3$, $R^2 = CH_2CH_3$

$C_{25}H_{28}O_8$ M 456.491
Constit. of *Hypericum drummondii*. Antimicrobial and cytotoxic agent. Yellow cryst. (hexane). Mp 136-138°.

Jayasuriya, H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 325 (*isol*, *pmr*, *cmr*)

Drummondin C **D-80532**

[119171-78-7]

As Drummondin A, D-80530 with

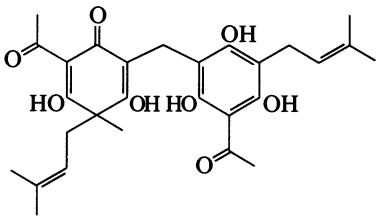
$R^1 = R^2 = CH_3$

$C_{24}H_{26}O_8$ M 442.465
Constit. of *Hypericum drummondii*. Antimicrobial and cytotoxic agent. Yellow cryst. (EtOAc). Mp 184-187°.

Jayasuriya, H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 325 (*isol*, *pmr*, *cmr*)

Drummondin F **D-80533**

[122127-73-5]



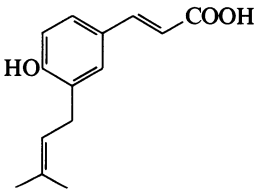
$C_{28}H_{34}O_8$ M 498.572
Constit. of *Hypericum drummondii*. Antimicrobial and cytotoxic agent. Yellow cryst. (hexane). Mp 106-107°. $[\alpha]_D$ +56.4° (c, 2.5 in MeOH).

Jayasuriya, H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 325 (*isol*, *pmr*, *cmr*)

Drupanin **D-80534**

3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenoic acid, 9CI. 4-Hydroxy-2-prenylcinnamic acid

[53755-58-1]

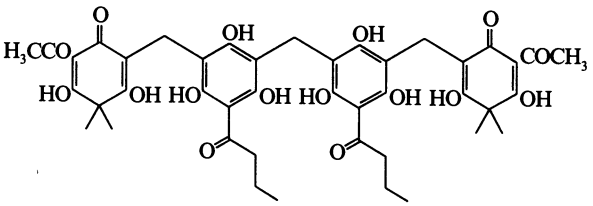


$C_{14}H_{16}O_3$ M 232.279
Constit. of the fruits of *Psoralea drupaecea*. Acicular cryst. Mp 147-148°.

Golovina, L.A. *et al*, *Khim. Prir. Soedin.*, 1973, **9**, 700; *cnc*, 672 (*isol*, *uv*, *pmr*, *struct*)

Dryocrassin **D-80535**

[12777-70-7]

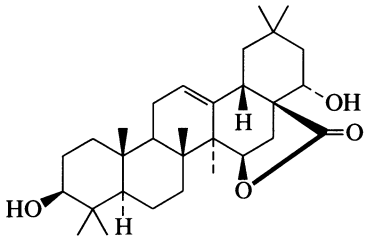


$C_{43}H_{48}O_{16}$ M 820.843

Isol. from *Dryopteris crassirhizoma* and *D. polylepis*. Yellow cryst. (Me_2CO). Mp 209-214°.

Noro, Y. *et al*, *Phytochemistry*, 1973, **12**, 1491 (*isol, uv, pmr, struct, synth*)

Dumortierigenin D-80536



$C_{30}H_{46}O_4$ M 470.691

Isol. from the cactus *Lemaireocereus dumortieri*. Cryst. (EtOH). Mp 292-295°. $[\alpha]_D^{30}$ −18.6° ($CHCl_3$).

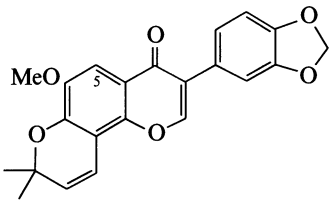
Djerassi, C. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2969; 1956, **78**, 5685 (*isol, struct*)

Shamma, M. *et al*, *J. Org. Chem.*, 1962, **27**, 4512 (*pmr*)

Durmillone D-80537

Updated Entry replacing D-08685

[24211-35-6]



$C_{22}H_{18}O_6$ M 378.381

Obt. from seeds of *Millettia dura*. Also from *M. ferruginea* and *m. rubiginosa*. Fine needles (MeOH). Mp 182-185°.

5-Methoxy: ***5-Methoxydurmillone***

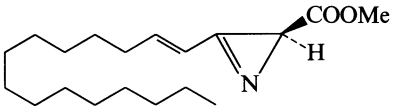
$C_{23}H_{20}O_7$ M 408.407

Constit. of *Millettia ferruginea*. Needles (MeOH). Mp 142-143°.

Ollis, W.D. *et al*, *Tetrahedron*, 1967, **23**, 4741 (*isol*)
Highet, R.J. *et al*, *J. Org. Chem.*, 1967, **32**, 1055 (*isol, struct*)
Krishnamurthi, M. *et al*, *Indian J. Chem.*, 1972, **10**, 914 (*synth*)
Desai, H.K. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 291 (*isol*)
Dagne, E. *et al*, *Phytochemistry*, 1989, **28**, 1897 (*derivs*)

Dysidazirine D-80538

[113507-74-7]



$C_{19}H_{33}NO_2$ M 307.475

Isol. from Fijian marine sponge, *Dysidea fragilis*. Low melting solid. $[\alpha]_D$ −165° (c, 0.5 in MeOH).

▷ Cytotoxic.

Molinski, T.F. *et al*, *J. Org. Chem.*, 1988, **53**, 2103 (*isol, uv, pmr, ms, abs config*)

Dysoxysulfone D-80539

$MeSO_2CH_2—S—S—CH_2—S—CH_2SO_2Me$

$C_5H_{12}O_4S_5$ M 296.477

Constit. of leaves of *Dysoxylum richii*. Shows antibiotic props. Prisms ($CHCl_3$). Mp 97-99°.

Jogia, M.K. *et al*, *Tetrahedron Lett.*, 1989, **30**, 4919 (*cryst struct*)

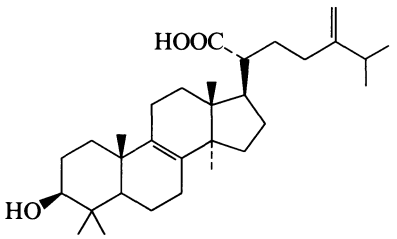
E

Eburicoic acid **E-80001**

Updated Entry replacing E-00002

3β-Hydroxy-24-methylene-8-lanosten-21-oic acid. Eburicolic acid

[560-66-7]



$C_{31}H_{50}O_3$ M 470.734

Constit. of *Polyporus* spp., *Lenzites* spp., *Fomes officinalis* and other fungi. Cryst. ($CHCl_3$/EtOH). Mp 292-293°. $[\alpha]_D^{17}$ +34° (c, 1.2 in Py).

Ac:

$C_{33}H_{52}O_4$ M 512.771

Constit. of *P. anthracophilus*. Cryst. Mp 259°. $[\alpha]_D^{19}$ +42° (c, 0.42 in $CHCl_3$).

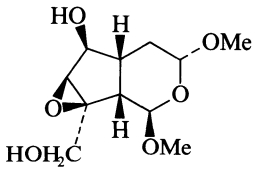
Me ester: [1259-85-4].

$C_{32}H_{52}O_3$ M 484.761

Constit. of *Basidiomycetes* spp. Cryst. (EtOAc). Mp 146-147°. $[\alpha]_D^{17}$ +45° (c, 1.8 in $CHCl_3$).

Holker, J.S.E. *et al*, *J. Chem. Soc.*, 1953, 2422 (*struct*)
Cohen, A.I. *et al*, *Tetrahedron*, 1965, **21**, 3171 (*pmr*)
Lawrie, W. *et al*, *J. Chem. Soc. C*, 1967, 2002 (*biosynth*)
Batey, I.L. *et al*, *Aust. J. Chem.*, 1972, **25**, 2511 (*isol*)
Yokoyama, A. *et al*, *Chem. Pharm. Bull.*, 1974, **22**, 877 (*isol*)

Eccremocarpol A **E-80002**

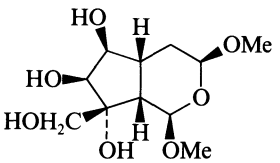


$C_{11}H_{18}O_6$ M 246.260

Constit. of *Eccremocarpus scaber*. Oil. $[\alpha]_D^{25}$ −29° (MeOH).

Garbarino, J.A. *et al*, *Heterocycles*, 1989, **28**, 697.

Eccremocarpol B **E-80003**



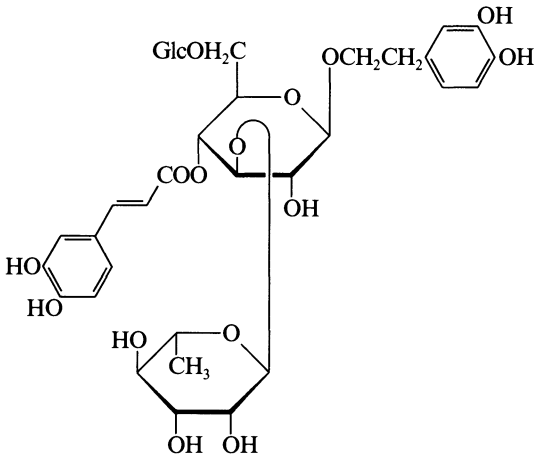
$C_{11}H_{20}O_7$ M 264.275

Constit. of *Eccremocarpus scaber*. Oil. $[\alpha]_D^{25}$ −18.5° (MeOH).

Garbarino, J.A. *et al*, *Phytochemistry*, 1989, **28**, 697.

Echinacoside **E-80004**

[82854-37-3]



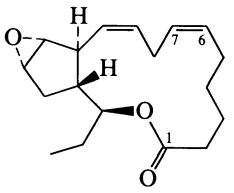
$C_{35}H_{46}O_{20}$ M 786.736

Isol. from roots of *Echinacea angustifolia* and from *Cistanche salsa*. Needles (EtOH). $[\alpha]_D^{20}$ −56.5° (H_2O).

Stoll, A. *et al*, *Helv. Chim. Acta*, 1950, **33**, 1877 (*isol*)
Becker, H. *et al*, *Z. Naturforsch., C*, 1982, **37**, 351 (*pmr*, *cmr*, *struct*)
Kobayashi, H. *et al*, *Chem. Pharm. Bull.*, 1984, **32**, 3009 (*isol*)

Ecklonialactone A **E-80005**

[121923-95-3]



$C_{18}H_{26}O_3$ M 290.402

Metab. of brown alga *Ecklonia stolonifera*. Cryst. (EtOH). Mp 96-98°. $[\alpha]_D$ −87.7° (c, 1.02 in $CHCl_3$).

6,7-Dihydro: [121923-96-4]. ***Ecklonialactone B***

$C_{18}H_{28}O_3$ M 292.417

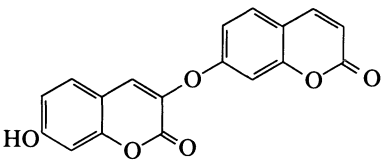
Metab. of *E. stolonifera*. Cryst. (EtOH). Mp 64-66°. $[\alpha]_D$ −49.3° (c, 1.08 in $CHCl_3$).

Kurata, K. *et al*, *Chem. Lett.*, 1989, 267 (*cryst struct*)

Edgeworin **E-80006**

3-(7-Coumarinyloxy)-7-hydroxycoumarin

[120028-43-5]



$C_{18}H_{10}O_6$ M 322.273

Constit. of *Edgeworthia chrysantha*. Powder. Mp 284-296° dec.

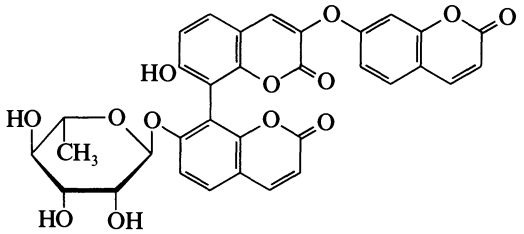
Ac: Cryst. (EtOAc/hexane). Mp 236-238°.

Baba, K. *et al*, *Phytochemistry*, 1989, **28**, 221.

Edgeworoside *A* E-80007

3-(7-Coumarinyloxy)-8-(7-hydroxycoumarin-8-yl)-7-α-L-rhamnopyranosyloxycoumarin

[120040-21-3]



$C_{33}H_{24}O_{13}$ M 628.545

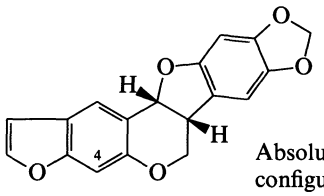
Constit. of *Edgeworthia chrysantha*. Powder. Mp 208-209°.

Baba, K. *et al*, *Phytochemistry*, 1989, **28**, 221.

Edulin E-80008

Neodulin

[13401-64-4]



Absolute configuration

$C_{18}H_{12}O_5$ M 308.290

Pterocarpan numbering shown. Isol. from *Neorautanenia edulis*. Needles ($CHCl_3/Et_2O$). Mp 225°. $[\alpha]_D^{25}$ −265.3° ($CHCl_3$).

4-Methoxy: [10338-03-1]. ***Ficinin***

$C_{19}H_{14}O_6$ M 338.316

Isol. from *N. ficifolia*. Cryst. Mp 180-180.5°. $[\alpha]_D^{20}$ −199.7°. No abs. config. assigned; given here by prob. analogy with Edulin.

Van Duuren, B.L., *J. Org. Chem.*, 1961, **26**, 5013 (*isol, uv, ir, pmr, struct*)

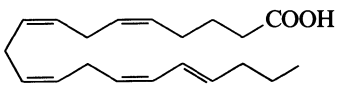
Itô, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1965, 595 (*abs config*)

Suginome, H., *Bull. Chem. Soc. Jpn.*, 1966, **39**, 1544 (*abs config*)

Brink, C. *et al*, *J. S. Afr. Chem. Inst.*, 1966, **19**, 24; *ca*, **65**, 13677 (*Ficinin*)

5,8,11,14,16-Eicosapentaenoic acid, 9CI E-80009

5,8,11,14,16-Icosapentaenoic acid. 16,17-Dehydroarachidonic acid



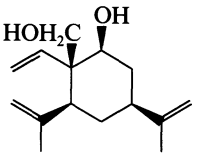
$C_{20}H_{30}O_2$ M 302.456

(5Z,8Z,11Z,14Z,16E)-form

Substrate for soybean lipoxygenase.

Corey, E.J. *et al*, *Tetrahedron Lett.*, 1987, **28**, 5391 (*synth, uv, ms*)

1,3,11-Elematriene-9,14-diol E-80010



$C_{15}H_{24}O_2$ M 236.353

9β-form

Periplocadiol

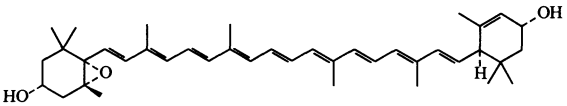
Constit. of *Periploea laevigata*. Oil. $[\alpha]_D$ −19° (c, 12.4 in $CHCl_3$).

Askri, M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 792 (*isol, pmr, cmr*)

Eloxanthin E-80011

5,6-Epoxy-5,6-dihydro-β,ε-carotene-3,3'-diol, 9CI. Xanthophyll epoxide. Lutein epoxide

[28368-08-3]

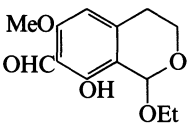


$C_{40}H_{56}O_3$ M 584.881

Isol. from a variety of higher plants and from algae. Orange cryst. (Et_2O/MeOH). Mp 192°. $[\alpha]_{644}^{18}$ +225° (C_6H_6).

Karrer, P. *et al*, *Helv. Chim. Acta*, 1945, **28**, 1146, 1526, 1528; 1946, **29**, 1539; 1947, **30**, 537, 1158, 1774; 1948, **31**, 113, 802; 1950, **33**, 300 (*isol, struct*)

Emehetin E-80012



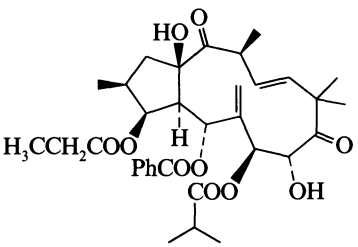
$C_{13}H_{16}O_5$ M 252.266

Metab. of *Emericella heterothallica*. Pale yellow cryst. (cyclohexane). Mp 109-110°. $[\alpha]_D^{25}$ −33.5° (c, 1.18 in $CHCl_3$).

Kawahara, N. *et al*, *Phytochemistry*, 1989, **28**, 1546.

Enukokurin E-80013

[122148-80-5]



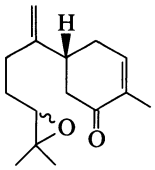
$C_{34}H_{44}O_{10}$ M 612.716

Constit. of *Euphorbia lateriflora*. Needles (Et_2O). Mp 193-195°. $[\alpha]_D^{25}$ +30.8° (c, 12.4 in $CHCl_3$).

Fakunle, C.O. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 279 (*isol, pmr, cmr*)

10,11-Epoxy-2,7(14)-bisaboladien-4-one E-80014

[119765-82-1]

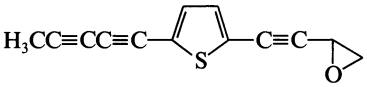


$C_{15}H_{22}O_2$ M 234.338
Constit. of *Mikania shushunensis*. Oil. $[\alpha]_D^{23}$ −18.9° (c, 2.1 in $CHCl_3$).

Gutierrez, A.B. *et al*, *Phytochemistry*, 1988, **27**, 3871.

2-(3,4-Epoxy-1-butynyl)-5-(1,3-pentadiynyl)thiophene, 8CI E-80015

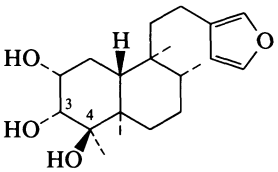
[1209-16-1]



$C_{13}H_8OS$ M 212.272
Isol. from roots of *Echinops sphaerocephalus*. Cryst. (pet. ether). Mp 54°. $[\alpha]_{546}^{25}$ +36° (c, 0.885 in Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 155, 876; 1968, **101**, 4163 (*isol, uv, ir, pmr, ord, struct, biosynth, synth*)

ent-15,16-Epoxy-13(16),14-clerodadiene-2β,3β,4α-triol E-80016



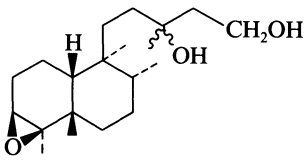
$C_{20}H_{32}O_4$ M 336.470
Constit. of *Baccharis boliviensis*. Cryst. Mp 155°. $[\alpha]_D^{24}$ +15° (c, 0.43 in $CHCl_3$).

4-Deoxy, 3-ketone: **ent-*15,16-Epoxy-2β-hydroxy-13(16),14-clerodadien-3-one***
$C_{20}H_{30}O_3$ M 318.455
Constit. of *B. boliviensis*. Gum.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

ent-3α,4α-Epoxy-13,15-clerodanediol E-80017

[118173-06-1]

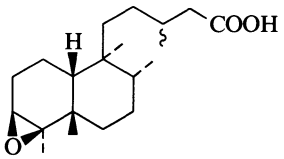


$C_{20}H_{36}O_3$ M 324.503
Constit. of *Ageratina saltillensis*.

Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187.

ent-3α,4α-Epoxy-15-clerodanoic acid E-80018

[118173-05-0]

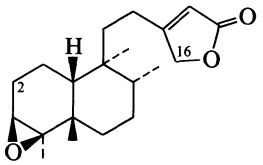


$C_{20}H_{34}O_3$ M 322.487
Constit. of *Ageratina saltillensis*.

Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187.

ent-3α,4α-Epoxy-13-cleroden-15,16-olide E-80019

[118243-67-7]



$C_{20}H_{30}O_3$ M 318.455
Constit. of *Solidago shortii*, *Ageratina cronquisti* and *A. saltillensis*. Cryst. Mp 91°.

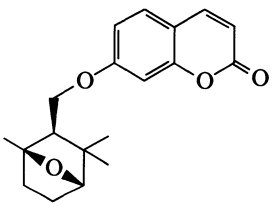
2β-Hydroxy: [118243-68-8]. ent-3α,4α-*Epoxy*-2α-*hydroxy*-13-*cleroden*-15,16-*olide*
$C_{20}H_{30}O_4$ M 334.455
Constit. of *A. saltillensis*.

16ξ-Hydroxy: [118172-98-8]. ent-3α,4α-*Epoxy*-16ξ-*hydroxy*-13-*cleroden*-15,16-*olide*
$C_{20}H_{30}O_4$ M 334.455
Constit. of *A. saltillensis*.

Anthonsin, T. *et al*, *Acta Chem. Scand.*, 1975, **25**, 1924 (*isol*)
Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187 (*isol, cryst struct*)

3′,6′-Epoxycycloauraptene E-80020

[21499-19-4]

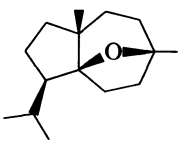


$C_{19}H_{22}O_4$ M 314.380
Isol. from *Aster yunnanensis*. Mp 187°. $[\alpha]_D$ +18.9° ($CHCl_3$).

(±)-*form* [31947-00-9]
Mp 155-156°.

Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1968, **717**, 186 (*isol*)
Coates, R.M. *et al*, *Tetrahedron*, 1970, **26**, 5699 (*synth*)

5,8-Epoxydaucane E-80021

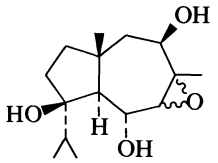


$C_{15}H_{26}O$ M 222.370
(*5β,8β*)-*form*

Carota-1,4β-oxide
Constit. of *Daucus carota*. Oil.

Dhillon, R.S. *et al*, *Phytochemistry*, 1989, **28**, 639.

7,8-Epoxy-4,6,9-daucanetriol E-80022

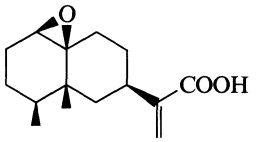


$C_{15}H_{26}O_4$ M 270.368

(4β,6α,7ξ,8ξ,9β)-form
2β-Hydroxy-3,4-epoxyjaeschkeanadiol
Constit. of *Ferula jaeschkeana*. Viscous mass. $[\alpha]_D$ +47° (c, 1.5 in $CHCl_3$).

Garg, S.N. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 771.

1,10-Epoxy-11(13)-eremophilen-12-oic acid E-80023

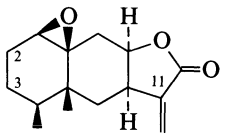


$C_{15}H_{22}O_3$ M 250.337

(1β,10β)-form
Oil.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

1,10-Epoxy-11(13)-eremophilen-12,8-olide E-80024



$C_{15}H_{20}O_3$ M 248.321

(1β,8β,10β)-form
Constit. of *Ondetia linearis*. $[\alpha]_D^{24}$ −17° (c, 3.68 in $CHCl_3$).

11α,13-Dihydro: 1β,10β-Epoxy-11αH-eremophilen-12,8β-olide
$C_{15}H_{22}O_3$ M 250.337
Constit. of *O. linearis*. Cryst. Mp 98°.

2α-Hydroxy: 1β,10β-Epoxy-2α-hydroxy-11(13)-eremophilen-12,8β-olide
$C_{15}H_{20}O_4$ M 264.321
Constit. of *O. linearis*. Gum.

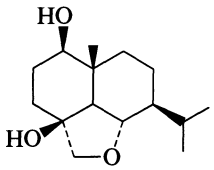
2α-Hydroxy, 11α,13-dihydro: 1β,10β-Epoxy-2α-hydroxy-11αH-eremophilen-12,8β-olide
$C_{15}H_{22}O_4$ M 266.336
Constit. of *O. linearis*. Cryst. Mp 145°. $[\alpha]_D^{24}$ −74° (c, 0.4 in $CHCl_3$).

2α-Hydroxy, 11β,13-dihydro: 1β,10β-Epoxy-2α-hydroxy-11βH-eremophilen-12,8β-olide
$C_{15}H_{22}O_4$ M 266.336
Constit. of *O. linearis*. Gum.

3α-Hydroxy, 11β,13-dihydro: 1β,10β-Epoxy-3α-hydroxy-11βH-eremophilen-12,8β-olide
$C_{15}H_{22}O_4$ M 266.336
Constit. of *O. linearis*. Gum.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

6,15-Epoxy-1,4-eudesmanediol E-80025

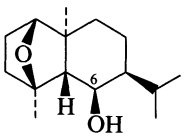


$C_{15}H_{26}O_3$ M 254.369

(1β,4β)-form [118243-71-3]
Constit. of *Ageratina saltillensis*.

Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187.

1,4-Epoxy-6-eudesmanol E-80026



$C_{15}H_{26}O_2$ M 238.369

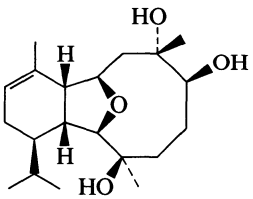
(1β,4β,5β,6β,10α)-form
6-Cinnamoyl: [119364-26-0]. *6α-Cinnamoyloxy-1β,4β-epoxy-1β,10α-eudesmane*
$C_{24}H_{32}O_3$ M 368.515
Constit. of *Ambrosia artemisioides*. Oil.

6-(4-Methoxybenzoyl): [119285-47-1]. *6α-Anisoyloxy-1β,4β-epoxy-1β,10α-eudesmane*
$C_{23}H_{32}O_4$
Constit. of *A. artemisioides*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551.

6,13-Epoxy-3-eunicellene-8,9,12-triol E-80027

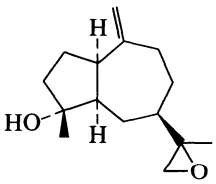
[123012-55-5]



$C_{20}H_{34}O_4$ M 338.486
Metab. of *Cladiella* sp. Prisms (CH_2Cl_2/hexane). Mp 205.5-206°. $[\alpha]_D$ −16.1° (c, 0.75 in $CHCl_3$). Cembrane numbering.

Uchio, Y. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3331 (*cryst struct*)

11,12-Epoxy-10(14)-guaien-4-ol E-80028



$C_{15}H_{22}O$ M 218.338

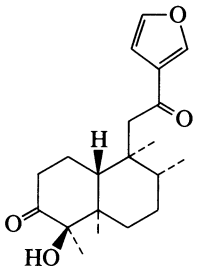
(1α,4α,5α)-form

Constit. of *Pleocarphus revolutus*. Oil. $[\alpha]_D^{24}$ +5° (c, 0.89 in $CHCl_3$).

Zdero, C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 509.

ent-15,16-Epoxy-4α-hydroxy-13(16),14-clerodadiene-3,12-dione **E-80029**

[118607-72-0]



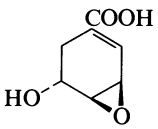
$C_{20}H_{28}O_4$ M 332.439

Constit. of *Croton argyrophylloides*. Cryst. (MeOH/hexane). Mp 122-124°. $[\alpha]_D^{25}$ +41° (c, 1.07 in $CHCl_3$).

Monte, F.J.Q. *et al*, *Phytochemistry*, 1988, **27**, 3209.

3,4-Epoxy-5-hydroxy-1-cyclohexene-carboxylic acid **E-80030**

5-Hydroxy-7-oxabicyclo[4.1.0]hept-2-ene-3-carboxylic acid. Anhydroshikimic acid



$C_7H_8O_4$ M 156.138

Me ester: [78961-89-4].

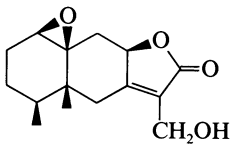
$C_8H_{10}O_4$ M 170.165

Metabolic of fungus *Chalara microspora*. Unstable oil. $[\alpha]_D$ +248° (c, 0.5 in EtOH).

[78844-86-7]

Fex, T. *et al*, *Acta Chem. Scand.*, *Ser. B*, 1981, **35**, 91 (*isol*)
Wood, H.B. *et al*, *Tetrahedron Lett.*, 1989, **30**, 6257 (*synth*)

1,10-Epoxy-13-hydroxy-7(11)-eremophilen-12,8-olide **E-80031**



$C_{15}H_{20}O_4$ M 264.321

(1β,8β,10β)-form

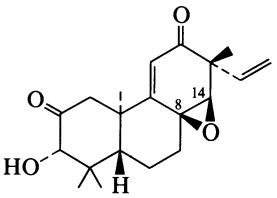
Constit. of *Ondetia linearis*. Cryst. Mp 129°. $[\alpha]_D^{24}$ −75° (c, 0.2 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

ent-8α,14α-Epoxy-3β-hydroxy-9(11),15-pimaradiene-2,12-dione **E-80032**

Yucalexin P-8

[119626-47-0]



$C_{20}H_{26}O_4$ M 330.423

Constit. of cassava roots (*Manihot esculenta*).

8,14-Diepimer: ent-8β,14β-*Epoxy*-3β-*hydroxy*-9(11),15-*pimaradiene*-2,12-*dione*. ***Yucalexin P-10***

$C_{20}H_{26}O_4$ M 330.423

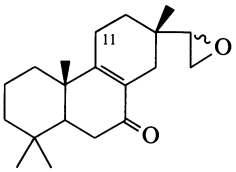
Constit. of *M. esculenta*.

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

15,16-Epoxy-8-isopimaren-7-one **E-80033**

Nanuzone

[120019-36-5]



$C_{20}H_{30}O_2$ M 302.456

Constit. of *Vellozia nanuzae*. Needles (hexane). Mp 132-134°. $[\alpha]_D$ +50° (c, 0.78 in $CHCl_3$).

11β-Hydroxy: [119944-13-7]. *15,16-Epoxy-11β-hydroxy*-8-*isopimaren*-7-*one*. ***11β-Hydroxynanuzone***

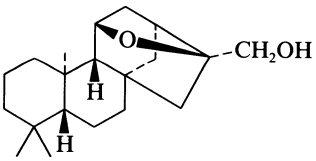
$C_{20}H_{30}O_3$ M 318.455

Constit. of *V. nanuzae*. Needles (EtOAc/hexane). Mp 149-151°.

Pinto, A.C. *et al*, *Phytochemistry*, 1988, **27**, 3909.

ent-11α,16α-Epoxy-17-kauranol **E-80034**

Liangshanin G

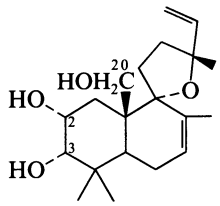


$C_{20}H_{32}O_2$ M 304.472

Constit. of *Rabdosia liangshanica*. Cryst. Mp 146-151°.

Fenglei, Z. *et al*, *Phytochemistry*, 1989, **28**, 1671.

9,13-Epoxy-7,14-labdadiene-2,3,20-triol E-80035



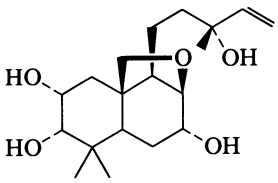
$C_{20}H_{32}O_4$ M 336.470

(2α,3α,9α,13R)-form

2-Angeloyl, 3,20-di-Ac: 3α,20-Diacetoxy-2α-angeloyloxy-9α,13R-epoxy-7,14-labdadiene
$C_{29}H_{42}O_7$ M 502.647
Constit. of *Waitzia acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

8,20-Epoxy-14-labdene-2,3,7,13-tetrol E-80036



$C_{20}H_{34}O_5$ M 354.486

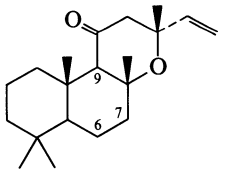
(2α,3α,7α,8β,13R)-form

2-Angeloyl: 2α-Angeloyloxy-8β,20-epoxy-14-labdene-3α,7α,13R-triol
$C_{25}H_{40}O_6$ M 436.587
Constit. of *Waitzia acuminata*.

2-Angeloyl, 3-Ac: 3α-Acetoxy-2α-angeloyloxy-8β,20-epoxy-14-labdene-7α,13R-diol
$C_{27}H_{42}O_7$ M 478.625
Constit. of *W. acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

8,13-Epoxy-14-labden-11-one E-80037



$C_{20}H_{32}O_2$ M 304.472

(8α,13R)-form [61242-47-5]
Constit. of *Coleus forskohlii*. Cryst. (2-propanol). Mp 96-97°. $[\alpha]_D^{20}$ −103.2° (c, 0.2 in CHCl).

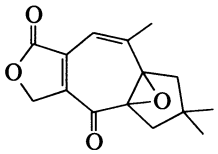
6β-Hydroxy: [121817-29-6]. ***8α,13R-Epoxy-6β-hydroxy-14-labden-11-one***
$C_{20}H_{32}O_3$ M 320.471
Constit. of *C. forskohlii*. Cryst. (EtOAc/cyclohexane). Mp 120-121°. $[\alpha]_D^{20}$ −133° (c, 0.1 in $CHCl_3$).

6β,7β,9α-Trihydroxy: [121606-18-6]. ***8α,13R-Epoxy-6β,7β,9-trihydroxy-14-labden-11-one***
$C_{20}H_{32}O_5$ M 352.470
Constit. of *C. forskohlii*. Cryst. (2-propanol). Mp 148-149°. $[\alpha]_D^{20}$ −25.9° (c, 0.1 in $CHCl_3$).

6β,9α-Dihydroxy,7β-acetoxy: [72963-77-0]. ***7β-Acetoxy-8α,13R-epoxy-6β,9α-dihydroxy-14-labden-11-one***
$C_{22}H_{34}O_6$ M 394.507
Constit. of *C. forskohlii*. Cryst. (hexane). Mp 135-136°. $[\alpha]_D^{20}$ −23.1° (c, 0.1 in $CHCl_3$).

Gabetta, B. *et al*, *Phytochemistry*, 1989, **28**, 859.

2,9-Epoxylactarotropone E-80038

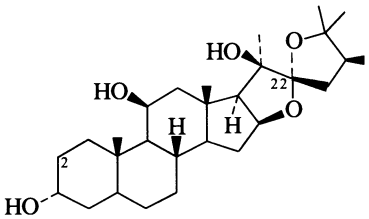


$C_{15}H_{16}O_4$ M 260.289
Constit. of *Lactarius scrobiculatus*. Oil.

Bosetti, A. *et al*, *Phytochemistry*, 1989, **28**, 1427.

22*S*,25-Epoxy-24-methyl-3,11,20-furostanetriol E-80039

Updated Entry replacing E-10055
Hippuristanol
[80442-78-0]



$C_{28}H_{46}O_5$ M 462.668
Constit. of *Isis hippuris*. Shows *in vivo* anticancer activity. Cryst. (MeOH). Mp 188-190°.

22-Epimer: [80442-79-1]. ***22-Epihippuristanol***
Constit. of *Isis hippuris*. Cryst. (MeOH). Mp 248-249°.

22-Epimer,di-Ac: [80442-84-8]. ***Hippurin-2***
$C_{32}H_{50}O_7$ M 546.743
Constit. of *I. hippuris*. Cryst. (MeOH). Mp 252-253°.

2α-Hydroxy: ***2α-Hydroxyhippuristanol***
$C_{28}H_{46}O_6$ M 478.668
Constit. of *I. hippuris*. Shows *in vivo* anticancer activity. Amorph. solid.

2α-Acetoxy: [66536-82-1]. ***Hippurin 1***
$C_{30}H_{48}O_7$ M 520.705
Constit. of *I. hippuris*. Cryst. (H_2O/pet. ether). Mp 183-185°. $[\alpha]_D$ +36.2° (c, 1 in $CHCl_3$).

2α-Acetoxy, 22-epimer: ***22-Epihippurin 1***
Constit. of *I. hippuris*. Cryst. (MeOH). Mp 243-245°.

2α,3,11-Di-Ac: ***3,11-Diacetylhippurin-1***
$C_{34}H_{52}O_9$ M 604.779
Constit. of *I. hippuris*. Oil.

2α-Hydroxy,22-epimer: ***2-Desacetyl-22-epihippurin 1***
$C_{28}H_{46}O_6$ M 478.668
Constit. of *I. hippuris*. Cryst. Mp 260-261°.

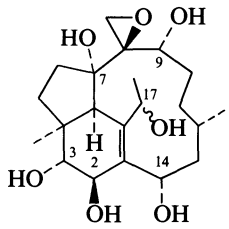
22-Epimer,2α-Hydroxy-3-Ac: ***3-Acetyl-2-desacetyl-22-epihippurin 1***
$C_{30}H_{48}O_7$ M 520.705
Constit. of *I. hippuris*. Cryst. Mp 248-250°.

22-Epimer,2α-acetoxy,3-Ac: ***3-Acetyl-22-epihippurin-1***
$C_{32}H_{50}O_8$ M 562.742
Constit. of *I. hippuris*. Cryst. Mp 240-243°.

22-Epimer,2α-Acetoxy,3,11-di-Ac: ***3,11-Diacetyl-22-epihippurin 1***
$C_{34}H_{52}O_9$ M 604.779
Constit. of *I. hippuris*. Needles. Mp 178-180°.

Kazlauskas, A. *et al*, *Tetrahedron Lett.*, 1977, 4439.
Higa, T. *et al*, *Chem. Lett.*, 1981, 1647.
Rao, C.B. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 954.

8,19-Epoxy-17-methyl-1(15)-trinervitene-2,3,7,9,14,17-hexol E-80040

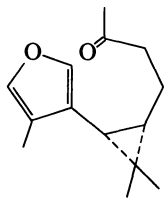


$C_{21}H_{34}O_6$ M 382.496
Unusual 17-methyltrinervitane skeleton.

(2β,3α,7α,8β,9α,14α)-form
2,3,9,14-Tetrapropanoyl:
$C_{35}H_{52}O_{12}$ M 664.789
Constit. of *Hospitalitermes umbrinus*. Gluey liquid.

Goh, S.H. *et al*, *Tetrahedron Lett.*, 1988, **29**, 113 (*struct*)

1,3-Epoxy-2-nor-1,10-seco-1(5),3-aromadendradien-10-one E-80041

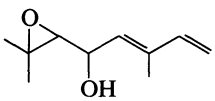


$C_{14}H_{20}O_2$ M 220.311
Constit. of *Mylia taylorii*. Oil. $[\alpha]_D$ −25.8° (c, 2.98 in $CHCl_3$).

Harrison, L.J. *et al*, *Phytochemistry*, 1989, **28**, 1261.

2,3-Epoxy-5,7-octadien-4-ol E-80042

6,7-Epoxy-5-hydroxyocimene
[119308-11-1]

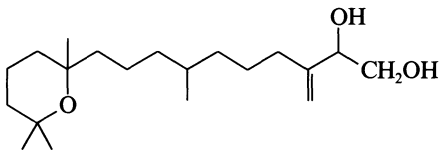


$C_{10}H_{16}O_2$ M 168.235
Constit. of *Cineraria britteniae*. Oil.

Lehmann, L. *et al*, *Phytochemistry*, 1988, **27**, 3307.

11,15-Epoxy-3(20)-phytene-1,2-diol E-80043

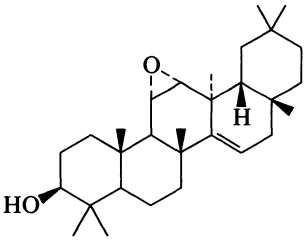
11,15-Epoxy-1,2-dihydroxy-3(20)-phytene



$C_{20}H_{38}O_3$ M 326.518
Constit. of *Anisopappus pinnatifidus*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1155.

11,12-Epoxy-14-taraxeren-3-ol E-80044



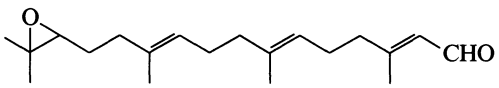
$C_{30}H_{48}O_2$ M 440.708

(3β,11α,12α)-form [3866-77-1] ***11α,12α-Oxidotaraxerol***
Constit. of *Euphorbia supina*. Needles (MeOH/$CHCl_3$). Mp 286-288°. $[\alpha]_D^{23}$ −38.9° (c, 0.98 in $CHCl_3$).

Tanaka, R. *et al*, *Phytochemistry*, 1988, **27**, 3579.

14,15-Epoxy-3,7,11,15-tetramethyl-2,6,10-hexadecatrienal E-80045

13-(3,3-Dimethyloxiranyl)-3,7,11-trimethyl-2,6,10-tridecatrienal, 9CI



(2*E*,6*E*,10*E*)-*form*

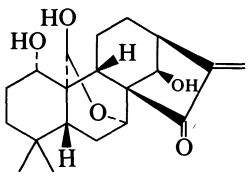
$C_{20}H_{32}O_2$ M 304.472

(2E,6E,10E)-form [108613-62-3]
Constit. of *Cystophora moniliformis*. Oil. $[\alpha]_D$ −17° (c, 0.98 in $CHCl_3$).

(2Z,6E,10E)-form [115075-54-2]
Constit. of *C. moniliformis*. Oil. $[\alpha]_D$ −22° (c, 0.4 in $CHCl_3$).

van Altena, I.A. *et al*, *Aust. J. Chem.*, 1988, **41**, 49.

ent-7β,20-Epoxy-1β,14α,20-trihydroxy-16-kauren-15-one E-80046

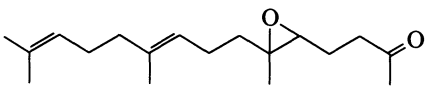


$C_{20}H_{28}O_5$ M 348.438
Constit. of *Rabdosia umbrosa*. Amorph. powder. $[\alpha]_D^{22}$ −55.8° (c, 1.54 in MeOH).

Takeda, Y. *et al*, *Phytochemistry*, 1989, **28**, 1691.

5,6-Epoxy-6,10,14-trimethyl-9,13-pentadecadien-2-one E-80047

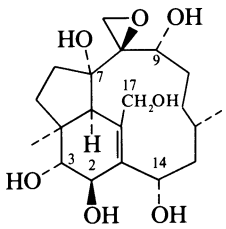
4-[3-(4,8-Dimethyl-3,7-nonadienyl)-3-methyloxiranyl]-2-butanone, 9CI
[115028-53-0]



$C_{18}H_{30}O_2$ M 278.434
Constit. of *Cystophora moniliformis*. Unstable oil.

van Altena, I.A., *Aust. J. Chem.*, 1988, **41**, 49.

8,19-Epoxy-1(15)-trinervitene-2,3,7,9,14,17-hexol E-80048



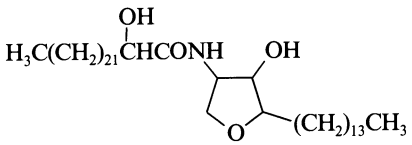
$C_{20}H_{32}O_7$ M 384.469

(2β,3α,7α,8β,9α,14α)-form

2,3,9,14,17-Pentapropanoyl:
$C_{35}H_{52}O_{12}$ M 664.789
Constit. of *Hospitalitermes umbrinus*. Gluey liquid.

Goh, S.H. *et al*, *Tetrahedron Lett.*, 1988, **29**, 113 (*struct*)

Ergocerebrin E-80049

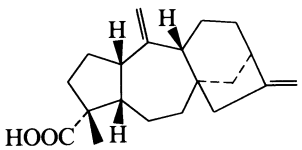


$C_{42}H_{83}NO_4$ M 666.122
Isol. from cultures of *Claviceps purpurea*. Needles. Mp 106-107°. $[\alpha]_D^{20}$ +16.3° (c, 0.17 in tetrachloroethane). Accompanied by its lower homologues with dodecyl and tridecyl sidechains.

Simon, J.W.A. *et al*, *J. Chem. Soc.*, 1965, 4164.

10(20),16-Ericacadien-19-oic acid E-80050

[122585-76-6]

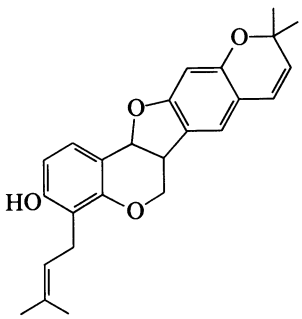


$C_{20}H_{28}O_2$ M 300.440
Constit. of *Helichrysum chionosphaerum*. Gum.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

Erybraedin D E-80051

[119269-72-6]

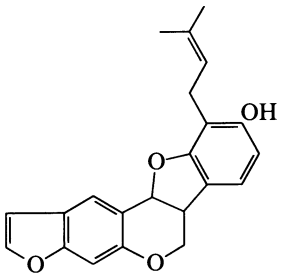


$C_{25}H_{26}O_4$ M 390.478
Constit. of *Erythrina mildbraedii*. $[\alpha]_D^{25}$ −67° (c, 0.23 in MeOH).

Mitscher, L.A. *et al*, *Heterocycles*, 1988, **27**, 2517.

Erybraedin E E-80052

[119269-73-7]



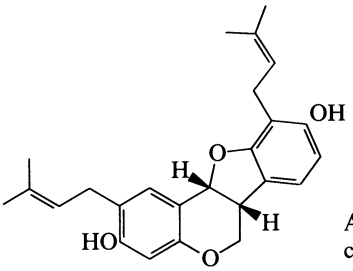
$C_{22}H_{20}O_4$ M 348.398
Constit. of *Erythrina mildbraedii*. $[\alpha]_D^{25}$ −104° (c, 0.29 in MeOH).

Mitscher, L.A. *et al*, *Heterocycles*, 1988, **27**, 2517.

Erythrabyssin II E-80053

3,9-Dihydroxy-2,10-diprenylcoumestan

[77263-06-0]



Absolute configuration

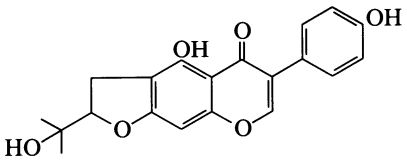
$C_{25}H_{28}O_4$ M 392.494
Isol. from roots of *Erythrina abyssinica*. Shows antimicrobial props.

Kamat, V.S. *et al*, *Heterocycles*, 1981, **15**, 1163 (*isol, uv, pmr, struct, abs config*)

Erythrinin C E-80054

2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-6-(4-hydroxyphenyl)-5H-furo[3,2-g][1]benzopyran-5-one, 9CI

[63807-85-2]

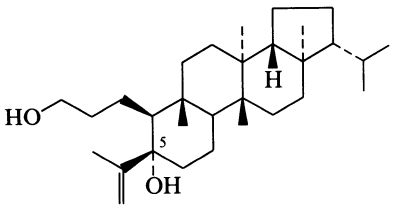


$C_{20}H_{18}O_6$ M 354.359
Isol. from bark of *Erythrina variegata*. Yellow needles (Me_2CO/C_6H_6). Mp 198°.

Deshpande, V.H. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 205.

Espinendiol A E-80055

3,4-Seco-D:B-friedo-B′:A′-neogammacer-4(23)-ene-3,5α-diol



$C_{30}H_{52}O_2$ M 444.740

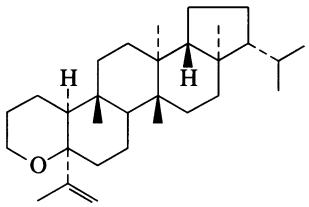
Constit. of *Euphorbia supina*. Cryst. Mp 194-196°. $[\alpha]_D^{23}$ +90.7° (c, 0.76 in $CHCl_3$).

5-Epimer: ***Espinendiol B.*** *3,4-Seco-D:B-friedo-B′:A′-neogammacer-4(23)-ene-3,5β-diol*
Constit. of *E. supina*. Cryst. Mp 192-193.5°. $[\alpha]_D^{23}$ −17.1° (c, 0.54 in $CHCl_3$).

Tanaka, R. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1661 (*cryst struct*)

Espinenoxide E-80056

3,4-Seco-D:B-friedo-B′:A′-neogammacer-4(23)-ene 3,5β-oxide

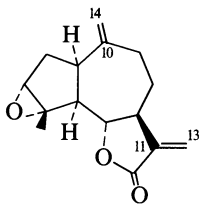


$C_{30}H_{50}O$ M 426.724
Constit. of *Euphorbia supina*. Cryst. Mp 215-218°. $[\alpha]_D^{23}$ +7.8° (c, 0.32 in $CHCl_3$).

Tanaka, R. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1661 (*cryst struct*)

Estafiatin E-80057

Updated Entry replacing E-10077
[10180-89-9]



$C_{15}H_{18}O_3$ M 246.305
Constit. of *Artemisia mexicana* and from *Cotula coronopifolia*. Cryst. (Et_2O/hexane). Mp 104-106°. $[\alpha]_D^{20}$ −9.9° ($CHCl_3$).

11α,13-Dihydro: ***11α,13-Dihydroestafialin.*** *3α,4α-Epoxy-10(14)-guaien-6α,12-olide*
$C_{15}H_{20}O_3$ M 248.321
Constit. of *A. sieversiana*. Oil. $[\alpha]_D^{24}$ +94° (c, 0.05 in $CHCl_3$).

10α,14-Epoxide: ***10α,14-Epoxyestafiatin***
$C_{15}H_{18}O_4$ M 262.305
Constit. of *Stevia alpina*. Cryst. (EtOAc/$CHCl_3$). Mp 113-119°.

10β,14-Epoxide: ***10β,14-Epoxyestafiatin***
$C_{15}H_{18}O_4$ M 262.305
Constit. of *S. alpina*. Cryst. (EtOAc/$CHCl_3$). Mp 159-161°.

Sánchez-Viesca, F. *et al*, *Tetrahedron*, 1963, **19**, 1285 (*isol, uv, ir, pmr*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2828 (*isol*)
Edgar, M.T. *et al*, *J. Org. Chem.*, 1979, **44**, 159 (*synth*)
Macaira, L.A. *et al*, *Tetrahedron Lett.*, 1980, 773 (*synth*)
Demuznek, M. *et al*, *Tetrahedron Lett.*, 1982, **23**, 2501 (*synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1985, **24**, 1009 (*isol*)
de Heluani, C.S. *et al*, *Phytochemistry*, 1989, **28**, 1931 (*isol, cryst struct*)

Ethenimine, 9CI E-80058

Vinylideneamine. Keteneimine
[17619-22-6]

$H_2C{=}C{=}NH$

C_2H_3N M 41.052
Transient species, rapidly tautomerizes to acetonitrile. Obs. at 14K and 77K.

Jacox, M.E., *Chem. Phys.*, 1979, **43**, 157 (*synth, ir, uv*)
Guillemin, J.-C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1983, 238 (*synth, ir*)
Rodler, M. *et al*, *Chem. Phys. Lett.*, 1984, **110**, 447 (*synth, bibl*)
Wentrup, C. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1337 (*props, bibl*)

3-Ethoxy-2-propenenitrile, 9CI E-80059

β-Ethoxyacrylonitrile
[61310-53-0]

EtOCH=CHCN

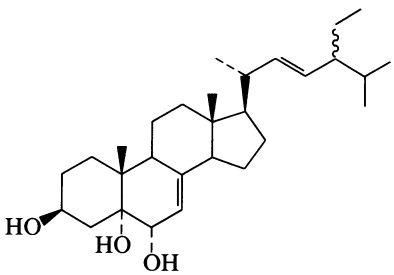
C_5H_7NO M 97.116
Inexpensive, comly. available synthetic reagent. Synthon for cytosines.

(E)-form [58243-08-6]
Liq. Bp_{15} 76-78°. n_D^{25} 1.4510.

(Z)-form [60036-64-8]
Liq. Bp_{15} 85-87°. n_D^{25} 1.4530.

McElvain, S.M. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 2657 (*synth, props*)
Scotti, F. *et al*, *J. Org. Chem.*, 1964, **29**, 1800 (*synth, ir, pmr, uv*)
Ford, G.P. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1975, 1371 (*synth, ir, props*)
Movsum-Zade, E.M. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1977, **13**, 1694 (*synth, ir*)
Smirnow, D. *et al*, *Synth. Commun.*, 1986, **16**, 1187 (*use*)

24-Ethyl-7,22-cholestadiene-3,5,6-triol E-80060

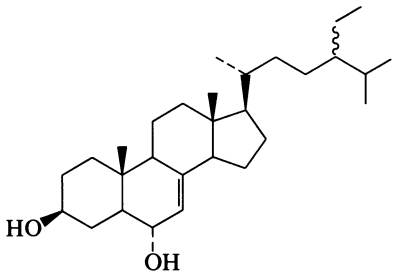


$C_{29}H_{48}O_3$ M 444.696

(3β,5α,6α,22E,24ξ)-form
Constit. of *Hippospongia communis*, *Spongia officinalis* and *Ircinia variabilis*.

Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol, pmr*)

24-Ethyl-7-cholestene-3,6-diol E-80061



$C_{29}H_{50}O_2$ M 430.713

(3β,5α,6α,24ξ)-form

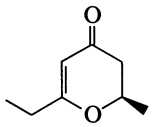
Constit. of *Spongionella gracilis*.

Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol*, *pmr*)

6-Ethyl-2,3-dihydro-2-methyl-4*H*-pyran-4-one E-80062

Updated Entry replacing E-50071

[96998-54-8]



$C_8H_{12}O_2$ M 140.182

(R)-form

Component of pheromone of male swift moth *Hepialus hecta*. Bp_{20} 105°. $[\alpha]_D^{22}$ +189° (c, 2.1 in pentane).

Sinnwell, V. *et al*, *Tetrahedron Lett.*, 1985, **26**, 1707 (*isol*)
Descheneaux, P.F. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1259 (*synth*, *pmr*, *bibl*)

Ethyl ethoxyiminoacetate, 9CI E-80063

Ethyl 1-carboethoxyformimidate

[816-27-3]

HN=C(OEt)COOEt

$C_6H_{11}NO_3$ M 145.158

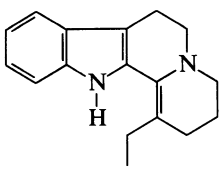
Reagent for heterocyclic synthesis. Liq. Bp 175° dec. , Bp_{18} 73°.

Lander, G.D., *J. Chem. Soc.*, 1895, **79**, 202; 1899, **83**, 411 (*synth*)
Cornforth, J.W. *et al*, *J. Chem. Soc.*, 1947, 96 (*synth*)
Braz, G.I. *et al*, *Zh. Obshch. Khim.*, 1964, **34**, 2980 (*synth*)
Sugiyama, Y. *et al*, *J. Org. Chem.*, 1978, **43**, 4485 (*use*)
Gomez, E. *et al*, *Tetrahedron*, 1986, **42**, 2625 (*use*)

1-Ethyl-2,3,4,6,7,12-hexahydroindolo[2,3-*a*]quinolizine, 9CI E-80064

Wenkert's enamine

[40163-47-1]



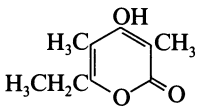
$C_{17}H_{20}N_2$ M 252.358

Key intermed. for eburnane alkaloid synth.

B,HClO₄: Mp 175-177°.

Wenkert, E. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 1580 (*synth*)
Husson, H.P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1972, 930 (*synth*)
Chevolot, L. *et al*, *Bull. Soc. Chim. Fr.*, 1976, 1222 (*synth*)
Szantay, C. *et al*, *Tetrahedron*, 1977, **33**, 1803 (*synth*, *use*)
Danieli, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1980, 109 (*synth*, *uv*, *ir*)
Lounasmaa, M. *et al*, *Tetrahedron*, 1987, **43**, 2135 (*synth*)

6-Ethyl-4-hydroxy-3,5-dimethyl-2*H*-pyran-2-one E-80065



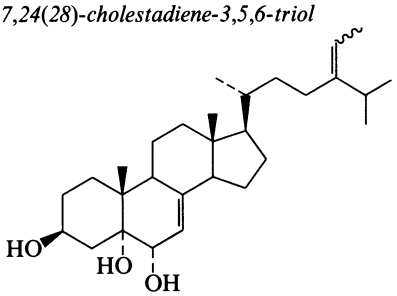
$C_9H_{12}O_3$ M 168.192

Metab. of *Emericella heterothallica*. Prisms (C_6H_6). Mp 152-154°.

Kawahara, N. *et al*, *Phytochemistry*, 1989, **28**, 1546.

24-Ethylidene-7-cholestene-3,5,6-triol E-80066

24-Ethyl-7,24(28)-cholestadiene-3,5,6-triol



$C_{29}H_{48}O_3$ M 444.696

(3β,5α,6α)-form

Constit. of *Hippospongia communis*, *Spongia officinalis*, and *Ircinia variabilis*.

Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol*, *pmr*)

3-Ethyl-1*H*-pyrrole E-80067

[1551-16-2]

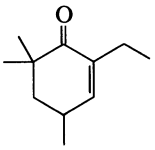
C_6H_9N M 95.144

Liq. Bp_{34} 88°. The 3-ethylpyrrole descr. in the old lit. is said to be the 2-isomer.

Fischer, H. *et al*, *Justus Liebigs Ann. Chem.*, 1935, **519**, 1 (*synth*)
Soth, S. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2511 (*synth*, *pmr*)
Alonso Garrido, D.O. *et al*, *J. Org. Chem.*, 1988, **53**, 403 (*synth*, *cmr*, *ms*)

2-Ethyl-4,6,6-trimethyl-2-cyclohexen-1-one E-80068

Angustifolenone



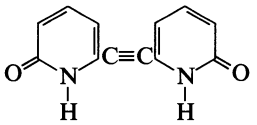
$C_{11}H_{18}O$ M 166.263

Constit. of *Backhousia angustifolia*. Oil.

Brophy, J.J. *et al*, *Phytochemistry*, 1989, **28**, 1259.

6,6′-(1,2-Ethynediyl)bis-2(1*H*)-pyridinone, 9CI **E-80069**

[117068-70-9]



$C_{12}H_8N_2O_2$ M 212.207

Ducharme, Y. *et al*, *J. Org. Chem.*, 1988, **53**, 5387 (*synth*)

Ethynol, 9CI **E-80070**

Updated Entry replacing E-50084

Hydroxyacetylene

[32038-79-2]

HC≡COH

C_2H_2O M 42.037

Obt. as stable sp. in gas phase.

tert-*Butyl ether:* [89489-28-1]. tert-*Butoxyethyne. 2-(Ethynyloxy)-2-methylpropane*

$C_6H_{10}O$ M 98.144

Bp_{22} ~20°.

Adamantyl ether: [113279-41-7]. *(1-Adamantyloxy)ethyne. 1-(Ethynyloxy)adamantane*

$C_{12}H_{16}O$ M 176.258

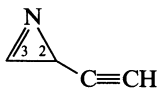
Cryst. (Et_2O/pentane). Mp 49-51°.

van Baar, B. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1986, **25**, 282 (*synth, ms*)

Pericàs, M.A. *et al*, *Tetrahedron*, 1987, **43**, 2311 (*deriv, synth, ir, pmr, cmr, ms*)

2-Ethynyl-2*H*-azirine **E-80071**

[119720-93-3]



C_4H_3N M 65.074

Kurtz, P. *et al*, *Justus Liebigs Ann. Chem.*, 1959, **624**, 1 (*synth*)

Banert, K., *Chem. Ber.*, 1989, **122**, 1175 (*synth, pmr, cmr*)

3-Ethynyl-2*H*-azirine **E-80072**

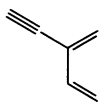
[119720-91-1]

C_4H_3N M 65.074

Banert, K., *Chem. Ber.*, 1989, **122**, 1175 (*synth, pmr, cmr*)

2-Ethynyl-1,3-butadiene **E-80073**

[6929-96-0]



C_6H_6 M 78.113

Extremely mobile liq. Bp 72°. n_D^{20} 1.4669 Dec. slowly at r.t.

Hopf, H., *Chem. Ber.*, 1971, **104**, 1499 (*synth, uv, pmr*)

Bader, H. *et al*, *Chem. Ber.*, 1989, **122**, 1193 (*synth, bibl*)

4-Ethynylindole **E-80074**

[102301-81-5]

$C_{10}H_7N$ M 141.172

Cryst. (EtOAc/hexane). Mp 66-66.5°.

Kozikowski, A.P. *et al*, *J. Org. Chem.*, 1988, **53**, 863 (*synth, ir, pmr, ms*)

Ethynylpentafluorobenzene **E-80075**

Updated Entry replacing E-70053

(Pentafluorophenyl)acetylene

[5122-07-6]

$(C_6F_5)C{\equiv}CH$

C_7HF_5 M 180.077

Liq. Bp 130-131°, Bp_{37} 50-52°.

▷ Potentially explosive.

Coe, P.L. *et al*, *J. Chem. Soc. C*, 1966, 597 (*synth, uv, ir, pmr*)

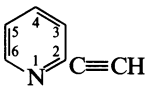
Waugh, F. *et al*, *J. Organomet. Chem.*, 1972, **39**, 275 (*synth, uv, ir, pmr*)

Neenan, T.X. *et al*, *J. Org. Chem.*, 1988, **53**, 2489 (*synth, ir, pmr, haz*)

2-Ethynylpyridine, 9CI **E-80076**

(2-Pyridyl)acetylene

[1945-84-2]



C_7H_5N M 103.123

Liq. Bp_{14} 77-78°. n_D^{21} 1.553.

Haug, V. *et al*, *Chem. Ber.*, 1960, **93**, 593 (*synth*)

Leaver, D. *et al*, *J. Chem. Soc.*, 1963, 6053 (*synth*)

Brandsma, L., *Prep. Acetylenic Chem.*, Elsevier, Amsterdam, 1971, 117 (*synth*)

Ames, D.E. *et al*, *Synthesis*, 1981, 364 (*synth*)

Sakamoto, T. *et al*, *Synthesis*, 1983, 312 (*synth, ir, pmr*)

3-Ethynylpyridine, 9CI **E-80077**

[2510-23-8]

C_7H_5N M 103.123

Cryst. (ligroin). Mp 38.5°. Bp_{30} 83-84°.

N-*oxide:* [49836-11-5].

C_7H_5NO M 119.123

Mp 104.5-105°.

Alberts, A. *et al*, *J. Am. Chem. Soc.*, 1935, **57**, 1286 (*synth*)

Kozhevnikova, A.N., *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1973, 1168 (*oxide*)

4-Ethynylpyridine, 9CI **E-80078**

(4-Pyridyl)acetylene

[2510-22-7]

C_7H_5N M 103.123

Cryst. (pentane). Mp 96-96.5°. Bp_{15} 70° subl.

N-Oxide: [49836-10-4].

C_7H_5NO M 119.123

No Mp reported.

Haug, U. *et al*, *Chem. Ber.*, 1960, **93**, 593 (*synth*)

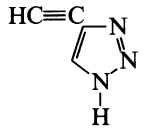
Gray, A.P. *et al*, *J. Org. Chem.*, 1968, **33**, 3007 (*synth*)

Kozhevnikova, A.N. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1973, 1168 (*oxide*)

Della Ciana, L. *et al*, *J. Heterocycl. Chem.*, 1984, **21**, 607 (*synth, pmr*)

4(5)-Ethynyl-1,2,3-triazole E-80079

[119720-87-5]

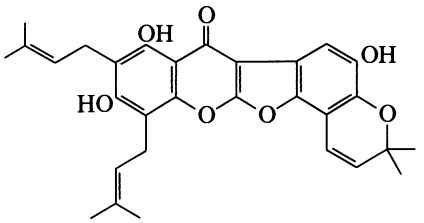


$C_4H_3N_3$ M 93.088
Solid (CH_2Cl_2 or by subl.). Mp 127.5°.

Banert, K., *Chem. Ber.*, 1989, **122**, 1175 (*synth, pmr, cmr*)

Euchretin A E-80080

[119459-83-5]

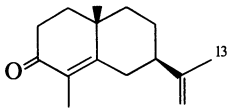


$C_{30}H_{30}O_7$ M 502.563
Constit. of *Euchresta japonica*. Pale yellow needles. Mp 208-209°.

Mizuno, M. *et al*, *Heterocycles*, 1988, **27**, 2047.

4,11-Eudesmadien-3-one E-80081

Updated Entry replacing C-03796
α-Cyperone
[473-08-5]



Absolute configuration

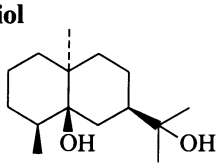
$C_{15}H_{22}O$ M 218.338
Constit. of *Cyperus rotundus*, *C. scariosus* and *Juniperus horizontalis*. Bp 177°. $[\alpha]_D$ +138°.

Semicarbazone: Cryst. Mp 216°.

13-Hydroxy: [56423-80-4]. *12-Hydroxy-4,11(13)-eudesmadien-3-one*. ***12-Hydroxy-α-cyperone***
$C_{15}H_{22}O_2$ M 234.338
Isol. from *Artemisia afra*. Oil.

Adamson, P.S. *et al*, *J. Chem. Soc.*, 1937, 1576 (*struct*)
Naves, Y.-R., *Bull. Soc. Chim. Fr.*, 1954, 332 (*isol*)
Howe, R. *et al*, *J. Chem. Soc.*, 1955, 2423 (*synth*)
Caine, D. *et al*, *J. Org. Chem.*, 1974, **39**, 2154 (*synth*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 1129 (*deriv*)

5,11-Eudesmanediol E-80082

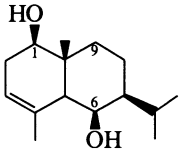


$C_{15}H_{28}O_2$ M 240.385
(4β,5β,7β,10α)-form [121817-19-4]
Constit. of *Cymbopogon distans*. Cryst. (Me_2CO). Mp 120-121°. $[\alpha]_D^{25}$ −9.0° (c, 0.8 in $CHCl_3$).

Mathela, C.S. *et al*, *Phytochemistry*, 1989, **28**, 936 (*isol, cryst struct*)

3-Eudesmene-1,6-diol E-80083

Updated Entry replacing E-01299
3-Selinene-1,6-diol



(1α,5α,6β,10β)-*form*

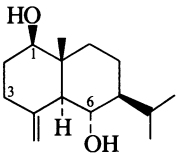
$C_{15}H_{26}O_2$ M 238.369
(1β,5α,6β,10β)-form
6-Cinnamoyl: [77355-61-4].
Constit. of *Solidago nemoralis*.
(1α,5β,6β,10α)-form
1-Cinnamoyl:
$C_{24}H_{32}O_3$ M 368.515
Constit. of *Ambrosia artemisioides*. Oil.
6-Cinnamoyl:
$C_{24}H_{32}O_3$ M 368.515
Constit. of *A. artemisioides*. Oil.
6-Anisoyl:
$C_{23}H_{32}O_4$ M 372.503
Constit. of *A. artemisioides*. Oil.
6-O-β-D-Glucopyranoside:
$C_{21}H_{36}O_7$ M 400.511
Constit. of *A. artemisioides*. Gum.

[77355-61-4]

Bohlmann, F. *et al*, *Phytochemistry*, 1980, **19**, 2655 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551 (*deriv*)

4(15)-Eudesmene-1,6-diol E-80084

Updated Entry replacing E-30080
1,6-Dihydroxy-4(15)-eudesmene



Absolute configuration

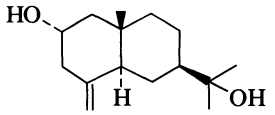
$C_{15}H_{26}O_2$ M 238.369
(1β,5α,6α,10β)-form
Constit. of *Senecio microglossus* and *Helianthus microcephalus*. Gum. $[\alpha]_D^{24}$ +7° (c, 0.1 in $CHCl_3$).
6-Me ether: 6α-Methoxy-4(15)-eudesmen-1β-ol. 1β-Hydroxy-6α-methoxy-4(15)-eudesmene
$C_{16}H_{28}O_2$ M 252.396
Constit. of *Torilis japonica*. Amorph. $[\alpha]_D$ +7.8°.
(1α,5β,6β,10α)-form
6-Angeloyl: 6β-Angeloyloxy-1α-hydroxy-5,10-bisepi-4(15)-eudesmene
$C_{20}H_{32}O_3$ M 320.471
Constit. of *Ambrosia artemisioides*. Oil.
6-Cinnamoyl, 3β-hydroperoxy: 6β-Cinnamoyloxy-3β-hydroperoxy-1α-hydroxy-5,10-bisepi-4(15)-eudesmene
$C_{24}H_{32}O_5$ M 400.514
Constit. of *A. artemisioides*. Oil.

Itokawa, H. *et al*, *Chem. Lett.*, 1983, 1253 (*isol*)
Bohlmann, F. *et al*, *Phytochemistry*, 1983, **22**, 1675 (*isol*)
Gutierrez, A.B. *et al*, *Phytochemistry*, 1988, **27**, 2225 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551 (*deriv*)

4(15)-Eudesmene-2,11-diol E-80085

Updated Entry replacing E-01301

4(15)-Selinene-2,11-diol



$C_{15}H_{26}O_2$ M 238.369

2α-form [21677-80-5] ***Pterocarpol***

Constit. of the heartwood of *Pterocarpus macrocarpus* and other *P.* spp. Cryst. (C_6H_6). Mp 104-105°. $[\alpha]_D$ +39° (c, 1.05 in $CHCl_3$).

Bahl, C.P. *et al*, *Tetrahedron*, 1968, **24**, 6231 (*isol, struct*)
Kukla, A.S. *et al*, *Indian J. Chem., Sect. B*, 1976, **14**, 905 (*abs config*)

3-Eudesmen-11-ol E-80086

Updated Entry replacing E-01309

α-Eudesmol. Selinelol. Atractylol. 3-Selinen-11-ol

[473-16-5]

$C_{15}H_{26}O$ M 222.370

Occurs with β-Eudesmol in various eucalyptus oils. Cryst. by subl. Mp 75°. Bp_{10} 156°. $[\alpha]_D$ +28.6° (c, 1.86 in $CHCl_3$).

7-Epimer: ***7-Epi-α-eudesmol***

$C_{15}H_{26}O$ M 222.370

Constit. of *Amyris balsamifera* oil. Oil.

McQuillan, F.J. *et al*, *J. Chem. Soc.*, 1956, 2973 (*isol, struct*)
Humber, D.C. *et al*, *Tetrahedron Lett.*, 1966, 4985 (*synth*)
Kutney, J.P. *et al*, *Can. J. Chem.*, 1984, **62**, 1407 (*synth*)
Schwartz, M.A. *et al*, *J. Org. Chem.*, 1985, **50**, 1359 (*synth*)
Van Beek, T.A. *et al*, *Phytochemistry*, 1989, **28**, 1909 (*isol*)

6-Eudesmen-4-ol E-80087

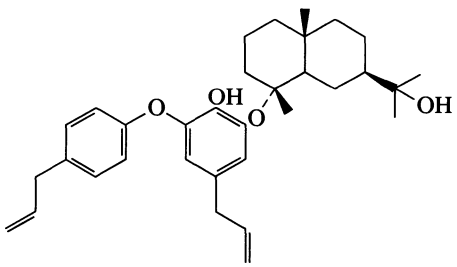
$C_{15}H_{26}O$ M 222.370

4α-form [118173-08-3]

Constit. of *Ageratina saltillensis*.

Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187.

Eudesobovatol A E-80088

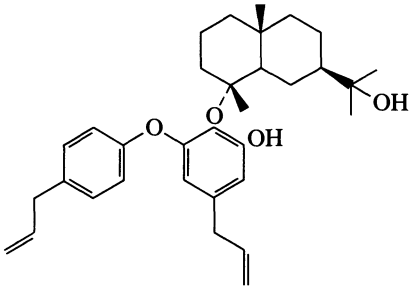


$C_{33}H_{44}O_4$ M 504.708

Constit. of *Magnolia obovata*. Neurotrophic agent. $[\alpha]_D$ −40.3° (c, 2.5 in $CHCl_3$).

Fukuyama, Y. *et al*, *Tetrahedron Lett.*, 1989, **30**, 5907.

Eudesobovatol B E-80089



$C_{33}H_{44}O_4$ M 504.708

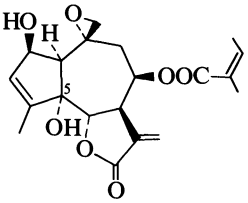
Constit. of *Magnolia obovata*. Neurotropic agent. $[\alpha]_D$ −26.1° (c, 1.15 in $CHCl_3$).

Fukuyama, Y. *et al*, *Tetrahedron Lett.*, 1989, **30**, 5907.

Euparotin E-80090

Updated Entry replacing E-01338

[10191-01-2]



$C_{20}H_{24}O_7$ M 376.405

Constit. of *Eupatorium rotundifolium*. Tumour growth inhibitor. Cryst. (EtOAc/pet. ether). Mp 199-200° (vac.). $[\alpha]_D^{32}$ −124° (c, 1.25 in EtOH).

Ac: [10215-89-1]. ***Euparotin acetate***

$C_{22}H_{26}O_8$ M 418.443

Constit. of *E. rotundifolium*. Tumour inhibitor. Cryst. ($CHCl_3/C_6H_6$/pet. ether). Mp 156-157° (vac.). $[\alpha]_D^{30}$ −191° (c, 0.54 in EtOH).

5-Deoxy: [89396-25-8]. ***5-Desoxyeuparotin***

$C_{20}H_{24}O_6$ M 360.406

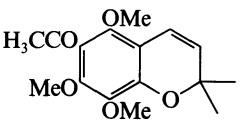
Constit. of *Trichogonia santosii*. Oil.

Kupchan, S.M. *et al*, *J. Org. Chem.*, 1969, **34**, 3876 (*struct, isol*)
Kupchan, S.M. *et al*, *J. Med. Chem.*, 1971, **14**, 1147 (*pharmacol*)
McPhail, A.T. *et al*, *Tetrahedron*, 1973, **29**, 1751 (*abs config*)
Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1984, 162 (*deriv*)

Evodione E-80091

1-(5,7,8-Trimethoxy-2,2-dimethyl-2H-1-benzopyran-6-yl)ethanone, 9CI. 6-Acetyl-5,7,8-trimethoxy-2,2-dimethyl-2H-1-benzopyran

[482-07-5]



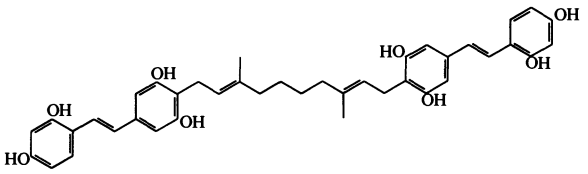
$C_{16}H_{20}O_5$ M 292.331

Isol. from leaves of *Evodia elleryana*. Mp 57°.

Wright, S.E., *J. Chem. Soc.*, 1948, 2005 (*struct*)
Huls, R. *et al*, *Bull. Soc. Chim. Belg.*, 1959, **68**, 325 (*synth*)
Barnes, C.S. *et al*, *Aust. J. Chem.*, 1964, **17**, 975 (*ms*)

Excelsaoctaphenol E-80092

[121747-80-6]

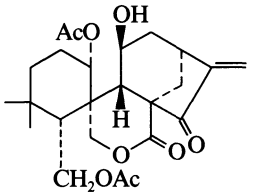


$C_{40}H_{42}O_8$ M 650.767

Constit. of *Chlorophora excelsa*. Light brown amorph. solid. Mp 210-216°.

Christensen, L.P. *et al*, *Phytochemistry*, 1989, **28**, 917.

Exidonin E-80093



$C_{24}H_{32}O_8$ M 448.512

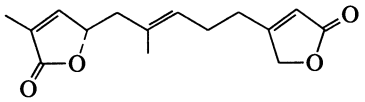
Constit. of *Rabdosia henryi*. Cryst. Mp 206-207°. $[\alpha]_D^{25}$ +101.6° (c, 0.37 in Py). A cleaved kaurane.

Meng, X. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 812.

F

2,6,10-Farnesatriene-1,15;13,9-diolide F-80001

*2-Methyl-5-[2-methyl-5-(5-oxo-2*H*-furan-3-yl)-2-pentenyl]-2(5*H*)-furanone*

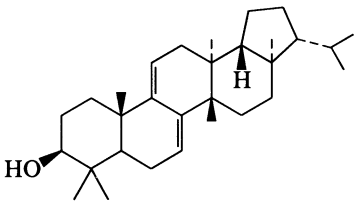


$C_{15}H_{18}O_4$ M 262.305

Compd. not named by authors. Constit. of *Eremophila miniata*. Amorph. solid. $[\alpha]_D$ +21.5° (c, 3 in $CHCl_3$).

Dastlik, K.A. *et al*, *Phytochemistry*, 1989, **28**, 1425.

7,9(11)-Fernadien-3-ol F-80002



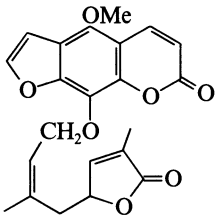
$C_{30}H_{48}O$ M 424.709

3β-form [53527-38-1]

Constit. of *Euphorbia supina*. Cryst. (MeOH/$CHCl_3$). Mp 193-196.5°.

Tanaka, R. *et al*, *Phytochemistry*, 1988, **27**, 3579.

Fernolin F-80003



$C_{22}H_{20}O_7$ M 396.396

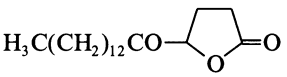
Constit. of *Fernonia limonia*. Cryst. Mp 262°.

Agrawal, A. *et al*, *Phytochemistry*, 1989, **28**, 1229.

Feronolide F-80004

*4,5-Dihydro-5-(1-oxotetradecyl)-2(3*H*)furanone. Dihydro-5-myristoyl-2(3*H*)-furanone, 8CI. 5-Oxo-4-octadecanolide*

[21566-75-6]



$C_{18}H_{32}O_3$ M 296.449

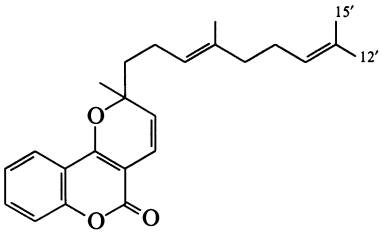
The proposed struct. (illus.) has been synthesised and was not identical with Feronolide. Currently the struct. of Feronolide is unknown. Isol. from cortex of *Feronia elephantum*. Cryst. (EtOH). Mp 115°. Mp. given refers to natural Feronolide. Synthetic compd. had Mp 66.5-68.5° (2,4-dinitrophenylhydrazone Mp. 61-63°).

Tiwari, R.D. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1964, **297**, 236.
Crundwell, E. *et al*, *J. Med. Chem.*, 1969, **12**, 547.

Ferprenin F-80005

Updated Entry replacing F-70003

[114727-96-7]



$C_{24}H_{28}O_3$ M 364.483

Constit. of *Ferula communis*. Oil. $[\alpha]_D^{25}$ +10° (c, 0.9 in $CHCl_3$).

12′-Hydroxy: ***(E)-ω-Hydroxyferprenin***
$C_{24}H_{28}O_4$ M 380.483
Constit. of *F. communis*. Yellow oil.

15′-Hydroxy: ***(Z)-ω-Hydroxyferprenin***
$C_{24}H_{28}O_4$ M 380.483
Constit. of *F. communis*. Yellow oil.

12′-Acetoxy: ***(E)-ω-Acetoxyferprenin***
$C_{26}H_{30}O_5$ M 422.520
Constit. of *F. communis*. Yellow oil.

15′-Acetoxy: ***(Z)-ω-Acetoxyferprenin***
$C_{26}H_{30}O_5$ M 422.520
Constit. of *F. communis*. Yellow oil.

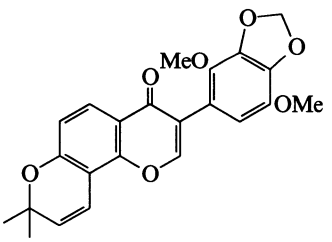
12′-Oxo: ***(E)-ω-Oxoferprenin***
$C_{24}H_{26}O_4$ M 378.467
Constit. of *F. communis*. Yellow oil.

Appendino, G. *et al*, *Phytochemistry*, 1988, **27**, 3619 (*deriv*)

Ferrugone F-80006

*3-(4,7-Dimethoxy-1,3-benzodioxol-5-yl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, 9CI*

[7731-08-0]



$C_{23}H_{20}O_7$ M 408.407

Isol. from *Millettia ferruginea* seeds. Needles (MeOH). Mp 167-169°.

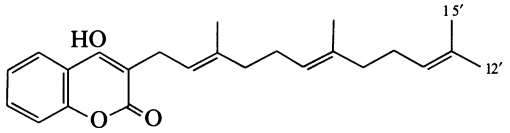
Highet, R.J. *et al*, *J. Org. Chem.*, 1967, **32**, 1055 (*isol, uv, ir, pmr, ms, struct*)

Ferulenol F-80007

Updated Entry replacing F-60005

4-Hydroxy-3-[(3,7,11-trimethyl-2,6,10-dodecatrienyl)]-2H-1-benzopyran-2-one, 9CI. 3-(1-Farnesyl)-4-hydroxycoumarin

[6805-34-1]



$C_{24}H_{30}O_3$ M 366.499

Constit. of the latex of *Ferula communis*. Shows haemorrhagic action. Mp 64-65°.

12′-Hydroxy: [106909-08-4]. ***(E)-ω-Hydroxyferulenol***

$C_{24}H_{30}O_4$ M 382.499

Constit. of *F. communis*. Shows haemorrhagic action. Yellow oil.

15′-Hydroxy: [110107-13-6]. ***(Z)-ω-Hydroxyferulenol***

$C_{24}H_{30}O_4$ M 382.499

Constit. of *F. communis* and *F. communis* var. *genuina*. Yellow oil.

12′-Acetoxy: [119234-02-5]. ***(E)-ω-Acetoxyferulenol***

$C_{26}H_{32}O_5$ M 424.536

Constit. of *F. communis*. Oil.

15′-Acetoxy: [119259-89-1]. ***(Z)-ω-Acetoxyferulenol***

$C_{26}H_{32}O_5$ M 424.536

Constit. of *F. communis*. Oil.

12′-Oxo: [106894-38-6]. ***(E)-ω-Oxoferulenol***

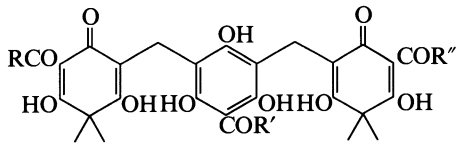
$C_{24}H_{28}O_4$ M 380.483

Constit. of *F. communis*. Oil.

Carboni, S. *et al*, *Tetrahedron Lett.*, 1964, 2783 (*struct, pmr*)
Lamnaouer, D. *et al*, *Phytochemistry*, 1987, **26**, 1613 (*isol, pmr, cmr*)
Valle, M.G. *et al*, *Phytochemistry*, 1987, **26**, 253 (*isol*)
Appendino, G. *et al*, *Phytochemistry*, 1988, **27**, 3619 (*derivs*)

Filixic acids F-80008

Updated Entry replacing F-20013



Filixic acid

ABA, R = R″ = CH_3, R′ = $CH_2CH_2CH_3$
ABP, R = CH_3, R′ = $CH_2CH_2CH_3$, R″ = CH_2CH_3
ABB, R = CH_3, R′ = R″ = $CH_2CH_2CH_3$
PBP, R = R″ = CH_2CH_3, R′ = $CH_2CH_2CH_3$
PBB, R = CH_2CH_3, R′ = R″ = $CH_2CH_2CH_3$
BBB, R = R′ = R″ = $CH_2CH_2CH_3$

The alphabetical suffixes refer to the acyl sustituents (A = acetyl, P = propionyl, B = butyryl). Isol. from ferns *Dryopteris* and *Aspidium* spp.

▷ LK4250000.

Filixic acid ABA [38226-84-5]

$C_{32}H_{36}O_{12}$ M 612.629

From *D. dickinsii*. Yellow needles (Me_2CO). Mp 163-166°.

Filixic acid ABP [57765-54-5]

$C_{33}H_{38}O_{12}$ M 626.656

Filixic acid ABB [37318-24-4]

$C_{34}H_{40}O_{12}$ M 640.683

Filixic acid PBP [51005-85-7]

$C_{34}H_{40}O_{12}$ M 640.683

Light-yellow needles (Me_2CO). Mp 192-194°. MF incorr. given as C_{30} by Hisada *et al.*

Filixic acid PBB [49582-09-4]

$C_{35}H_{42}O_{12}$ M 654.710

Mp 184-186°.

Filixic acid BBB [4482-83-1]

Filixic acid. Filicin

$C_{36}H_{44}O_{12}$ M 668.736

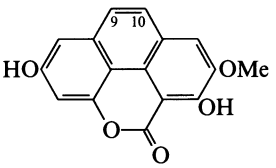
Cryst. (Me_2CO), light yellow tablets (EtOAc). Mp 184-185° (168-170°).

Penttila, A. *et al*, *Acta Chem. Scand.*, 1963, **17**, 191 (*isol, struct*)
Hisada, S. *et al*, *Phytochemistry*, 1972, **11**, 1850, 2881; 1973, **12**, 1493 (*isol*)
Lounasmaa, M. *et al*, *Helv. Chim. Acta*, 1973, **56**, 1133 (*ms*)
Widen, C.J. *et al*, *Planta Med.*, 1975, **28**, 144 (*isol*)
Lounasmaa, M., *Planta Med.*, 1978, **33**, 173 (*cmr*)

Flaccidinin F-80009

2,6-Dihydroxy-7-methoxy-5H-phenanthro[4,5-bcd]pyran-5-one, 9CI

[121817-23-0]



$C_{16}H_{10}O_5$ M 282.252

Constit. of *Coelogyne flaccida*. Cryst. (EtOAc/pet. ether). Mp 360° dec.

9,10-Dihydro: [121817-24-1]. ***Oxoflaccidin***

$C_{16}H_{12}O_5$ M 284.268

Constit. of *C. flaccida*.

9,10-Dihydro, deoxo: [115531-76-5]. ***Flaccidin***

$C_{16}H_{14}O_4$ M 270.284

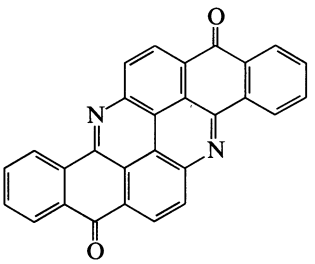
Constit. of *C. flaccida*. Cryst. ($CHCl_3$). Mp 200°.

Majumder, P.L. *et al*, *Phytochemistry*, 1988, **27**, 899; 1989, **28**, 887.

Flavanthrone, 8CI F-80010

Benzo[h]benz[5,6]acridino[2,1,9,8-klmna]acridine-8,16-dione, 9CI. C.I. Pigment Yellow 24. C.I. Vat Yellow 1

[475-71-8]



$C_{28}H_{12}N_2O_2$ M 408.415

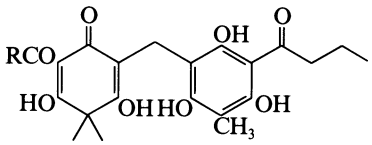
Dye, pigment, used in inks, paints, plastics and coloured textiles. Yellow-brown needles ($PhNO_2$ or by subl.). Green fluor. in cumene soln. Much patented.

Colour Index, **3**, 3274.
Krepelka, V. *et al*, *Collect. Czech. Chem. Commun.*, 1937, **9**, 29 (*synth*)
Stadler, H.P., *Acta Crystallogr.*, 1953, **6**, 540 (*cryst struct*)
Durie, R.A. *et al*, *Aust. J. Chem.*, 1957, **10**, 429 (*ir*)
Moran, J.J. *et al*, *J. Chem. Soc.*, 1957, 765 (*purifn, uv*)
Sramek, J., *J. Soc. Dyers Colour.*, 1962, **78**, 326 (*chromatog*)

Kratochvil, V. *et al*, *Collect. Czech. Chem. Commun.*, 1974, **39**, 2814 (*synth, uv*)
Kirk-Othmer Encycl. Chem. Technol., 3*rd Ed.*, 1978-1984, *Wiley, NY*, 3rd Ed., Wiley, N.Y., 1984, **8**, 242.

Flavaspidic acids F-80011

Updated Entry replacing F-00164



Flavaspidic acid AB, R = CH_3
PB, R = CH_2CH_3
BB, R = $CH_2CH_2CH_3$

The suffixes refer to the acyl substituents (A = acetyl, P = propionyl, B = butyryl). Isol. from ferns, esp. *Dryopteris* spp.

▷ EU1400000.

Flavaspidic acid AB [3761-64-6]
$C_{22}H_{26}O_8$ M 418.443
Mp 210-212°.

Flavaspidic acid PB [3773-25-9]
$C_{23}H_{28}O_8$ M 432.469
Mp 170-171°.

Di-Ac:
$C_{28}H_{34}O_{10}$ M 530.571
Mp 142-143°.

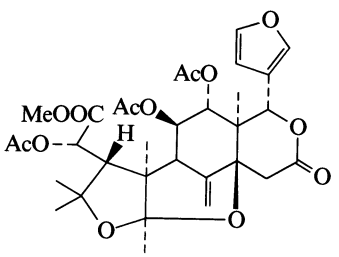
Flavaspidic acid BB [114-42-1]
Flavaspidic acid. Polystichocitrin. Toxifren
$C_{24}H_{30}O_8$ M 446.496
Yellow or colourless cryst. Mp 92°, Mp 156° (double Mp). The two forms are considered to be tautomers which interconvert on heating.

Di-Ac: Mp 142-143°.

McGookin, A. *et al*, *J. Chem. Soc.*, 1953, 1828 (*synth*)
Penttilä, A. *et al*, *Acta Chem. Scand.*, 1964, **18**, 344 (*isol, synth*)
Erämetsä, O. *et al*, *Acta Chem. Scand.*, 1970, **24**, 3335 (*cryst struct*)
Lounasmaa, M. *et al*, *Helv. Chim. Acta*, 1973, **56**, 1133 (*ms*)
Widén, C.-J. *et al*, *Helv. Chim. Acta*, 1976, **59**, 1725 (*isol, bibl*)
Lounasmaa, M., *Planta Med.*, 1978, **33**, 173 (*cmr*)

Flindercarpin 2 F-80012

[61903-01-3]

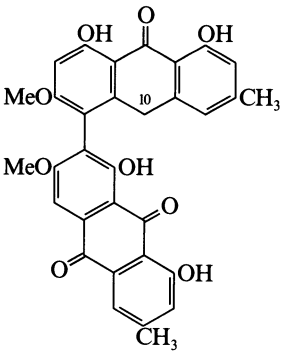


$C_{32}H_{40}O_{13}$ M 632.660
Isol. from the bark of *Flindersia laevicarpa*. Shows insect antifeedant activity. Mp 232°. The structs of Flindercarpin 1, $C_{25}H_{28}O_{11}$ and Flindercarpin 3, $C_{26}H_{32}O_9$ have not yet been detd.

Picker, K. *et al*, *Aust. J. Chem.*, 1976, **29**, 2023 (*isol*)
Breen, G.W. *et al*, *Aust. J. Chem.*, 1984, **37**, 1461 (*cryst struct*)

Floribundone 2 F-80013

[118555-83-2]



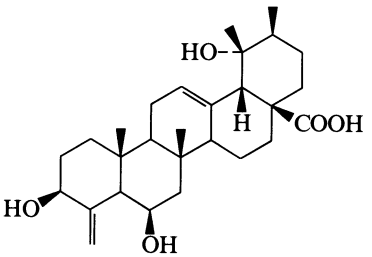
$C_{32}H_{24}O_9$ M 552.536
Constit. of leaves of *Cassia floribunda*.

10-Oxo: [118555-84-3]. ***Floribundone 1***
$C_{32}H_{22}O_{10}$ M 566.520
Orange cryst. (MeOH). Mp >260°. $[\alpha]_D^{18}$ +130° (c, 0.05 in $CHCl_3$).

Alemayehu, G. *et al*, *Phytochemistry*, 1988, **27**, 3255.

Floridic acid F-80014

3β,6β,19α-Trihydroxy-23-nor-4(24),12-ursadien-28-oic acid



$C_{29}H_{44}O_5$ M 472.664
Constit. of *Uncaria florida*.

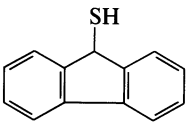
Me ester: Prisms (Me_2CO aq.). Mp 146-148°.

Aimi, N. *et al*, *Tetrahedron*, 1989, **45**, 4125.

9*H*-Fluorene-9-thiol F-80015

9-Fluorenylmercaptan. 9-Mercaptofluorene

[19552-08-0]



$C_{13}H_{10}S$ M 198.288
Plates (MeOH/AcOH). Mp 105-106°.

S-*Me:* [59431-17-3]. *9-(Methylthio)-9H-fluorene*
$C_{14}H_{12}S$ M 212.315
Cryst. (MeOH). Mp 46-47°.

S-*Me*, S-*oxide: 9-(Methylsulfinyl)-9H-fluorene*
$C_{14}H_{12}OS$ M 228.314
Mp 83-84°.

S-*Me*, S-*dioxide:* [31859-90-2]. *9-(Methylsulfonyl)-9H-fluorene*
$C_{14}H_{12}O_2S$ M 244.314
Long needles (MeOH or AcOH). Mp 188-189°.

S-*Ph:* [28114-92-3]. *9-(Phenylthio)-9H-fluorene*
$C_{19}H_{14}S$ M 274.386
Mp 48-49°.

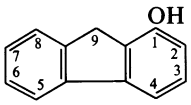
S-*Ph*, S-*oxide: 9-(Phenylsulfinyl)-9*H*-fluorene*
$C_{19}H_{14}OS$ M 290.385
Mp 104-105°.

S-*Ph*, S-*dioxide:* [22010-78-2]. *9-(Phenylsulfonyl)-9*H*-fluorene*
$C_{19}H_{14}O_2S$ M 306.384
Prisms (Me_2CO/heptane). Mp 182-183°.

Klerk, M.M. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 3846 (*synth*)
Bavin, P.M.G., *Can. J. Chem.*, 1960, **38**, 917; 1962, **40**, 220 (*deriv*)
Pan, H.-L. *et al*, *Chem. Ind. (London)*, 1968, 546 (*synth*)
Kice, J.L. *et al*, *J. Org. Chem.*, 1988, **53**, 3593 (*synth, pmr, deriv*)

9*H*-Fluoren-1-ol, 9CI F-80016

Updated Entry replacing F-00259
1-Hydroxyfluorene
[6344-61-2]



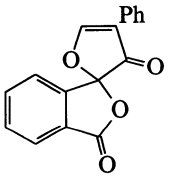
$C_{13}H_{10}O$ M 182.221
A quoted synthesis by Kumar *et al* (1983) is prob. erroneous. Mp 119.9-120.5°.

Me ether: [26060-14-0]. *1-Methoxyfluorene*
$C_{14}H_{12}O$ M 196.248
Mp 85-86°.

Weisburger, E.K. *et al*, *J. Org. Chem.*, 1953, **18**, 864 (*synth, derivs*)
Shapiro, M.J., *J. Org. Chem.*, 1978, **43**, 3769 (*nmr*)
Kumar, B. *et al*, *Synthesis*, 1983, 115 (*synth*)
Blokker, V. *et al*, *J. Org. Chem.*, 1988, **53**, 5567 (*synth*)

Fluorescamine F-80017

*4-Phenylspiro[furan-2(3*H*),1′(3′*H*)-isobenzofuran]-3,3′-dione, 9CI. 4-Phenylspiro[furan-2(3*H*),1′phthalan]-3,3′-dione. Fluram*
[38183-12-9]

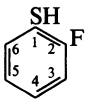


$C_{17}H_{10}O_4$ M 278.264
Reagent for fluorimetric assay of amino acids and primary amines. Cryst. (CH_2Cl_2/Et_2O). Mp 154-155°.

Weigele, M. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5927 (*synth*)
Undenfriend, S. *et al*, *Science (Washington, D.C.)*, 1972, **178**, 871 (*use*)
Weigele, M. *et al*, *Biochem. Biophys. Res. Commun.*, 1973, **50**, 352.
Weigele, M. *et al*, *J. Org. Chem.*, 1976, **41**, 388 (*synth, ir, uv*)
Undenfriend, S., *Pharmacology*, 1979, **19**, 223 (*rev, use*)
Doetsch, P.W. *et al*, *J. Chromatogr.*, 1980, **189**, 79 (*use, bibl*)
Merck Index, 10th Ed., 1983, 4059.

2-Fluorobenzenethiol, 9CI F-80018

1-Fluoro-2-mercaptobenzene. 2-Fluorothiophenol
[2557-78-0]



C_6H_5FS M 128.170
Bp_{15} 65°. n_D^{26} 1.5395.

Sharghi, N., *J. Chem. Eng. Data*, 1963, **8**, 276 (*synth*)
Cervena, I. *et al*, *Collect. Czech. Chem. Commun.*, 1979, **44**, 2139 (*synth*)

3-Fluorobenzenethiol, 9CI F-80019

1-Fluoro-3-mercaptobenzene. 3-Fluorothiophenol
[2557-77-9]
C_6H_5FS M 128.170
Bp 156°, Bp_{11} 53°. n_D^{27} 1.5481.

Taft, R.W., *J. Am. Chem. Soc.*, 1963, **85**, 709 (*pmr*)
Sharghi, N. *et al*, *J. Chem. Eng. Data*, 1963, **8**, 276 (*synth*)
Rajšner, M. *et al*, *Collect. Czech. Chem. Commun.*, 1967, **32**, 2021 (*synth*)
Cutress, N.C. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1974, 263 (*ir*)
Protiva, M. *et al*, *Collect. Czech. Chem. Commun.*, 1986, **51**, 2598 (*synth*)

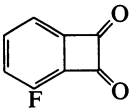
4-Fluorobenzenethiol, 9CI F-80020

1-Fluoro-4-mercaptobenzene. 4-Fluorothiophenol
[371-42-6]
C_6H_5FS M 128.170
Bp 162°, $Bp_{2.3}$ 29-30°. n_D^{25} 1.5485.

Oae, S. *et al*, *Tetrahedron Lett.*, 1972, 1283 (*synth*)
Cutress, N.C. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1974, 263 (*ir*)
Rajsner, M. *et al*, *Collect. Czech. Chem. Commun.*, 1975, **40**, 719 (*synth*)
Senoff, C.V. *et al*, *Inorg. Chem.*, 1975, **14**, 278 (*cmr*)
Pradip, H. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 7056 (*nmr*)

3-Fluorobenzocyclobutene-1,2-dione F-80021

2-Fluorobicyclo[4.2.0]octa-1,3,5-triene-7,8-dione
[118112-24-6]

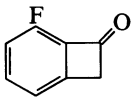


$C_8H_3FO_2$ M 150.109
Cryst. (hexane). Mp 95°.

Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, ir, pmr, cmr*)

6-Fluorobenzocyclobuten-1-one F-80022

5-Fluorobicyclo[4.2.0]octa-1,3,5-trien-7-one
[118112-20-2]

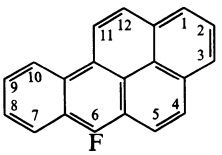


C_8H_5FO M 136.125
Cryst. by subl. Mp 39-42°.

Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1989, **54**, 1435 (*synth, ir, pmr, cmr*)

6-Fluorobenzo[*a*]pyrene F-80023

[59417-86-6]



$C_{20}H_{11}F$ M 270.305

Cryst. (Me_2CO/MeOH). Mp 167-169°.

Agranat, I. *et al*, *Experientia*, 1976, **32**, 417 (*synth*)
Cremonesi, P. *et al*, *J. Org. Chem.*, 1989, **54**, 3561 (*synth, pmr*)

7-Fluorobenzo[*a*]pyrene F-80024

[71511-38-1]

$C_{20}H_{11}F$ M 270.305
Yellow-green fluorescent cryst. (Et_2O/pet.ether). Mp 174-175°.

Paulsen, H. *et al*, *Chem. Ber.*, 1979, **112**, 2907 (*synth, uv, ir*)
Newman, M.S. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 6788 (*synth, pmr, F nmr*)
Sardella, D.J. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 287 (*cmr*)

8-Fluorobenzo[*a*]pyrene F-80025

[71171-92-1]

$C_{20}H_{11}F$ M 270.305
Cryst. by subl. Mp 167.5-168°.

Newman, M.S. *et al*, *J. Org. Chem.*, 1979, **44**, 3388 (*synth*)
Sardella, D.J. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 287 (*cmr*)

9-Fluorobenzo[*a*]pyrene F-80026

[71171-93-2]

$C_{20}H_{11}F$ M 270.305
Yellow-green fluorescent cryst. (Et_2O/pet.ether). Mp 157.5-158.5°.

Paulsen, H. *et al*, *Chem. Ber.*, 1979, **112**, 2907 (*synth, uv, ir*)
Newman, M.S. *et al*, *J. Org. Chem.*, 1979, **44**, 3388 (*synth*)
Sardella, D.J. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 287 (*cmr*)

10-Fluorobenzo[*a*]pyrene F-80027

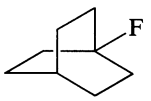
[74018-58-9]

$C_{20}H_{11}F$ M 270.305
Cryst. (C_6H_6/EtOH). Mp 152-153°.

Newman, M.S. *et al*, *Bull. Soc. Chim. Belg.*, 1979, **88**, 871 (*synth*)
Sardella, D.J. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 287 (*cmr*)

1-Fluorobicyclo[2.2.2]octane F-80028

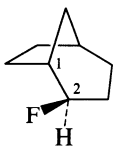
[20277-22-9]



$C_8H_{13}F$ M 128.189
Cryst. Mp 174° (182-184°). Mostly sublimes at 152°.

Suzuki, Z. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 1724 (*synth*)
Kopecky, J. *et al*, *Chem. Ind. (London)*, 1969, 271 (*synth*)
Maciel, G.E. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 1268 (*cmr*)
Rozen, S. *et al*, *J. Org. Chem.*, 1988, **53**, 2803 (*synth*)

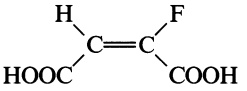
2-Fluorobicyclo[3.2.1]octane F-80029



$C_8H_{13}F$ M 128.189
(*1RS,2RS*)-*form* [114423-47-1]
(±)-exo-*form*
Cryst. (pentane/MeOH). Mp 131°.

Rozen, S. *et al*, *J. Org. Chem.*, 1988, **53**, 2803 (*synth, pmr, F nmr, cmr*)

2-Fluoro-2-butenedioic acid, 9CI F-80030



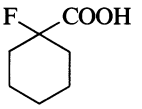
(*E*)-*form*

$C_4H_3FO_4$ M 134.064
(*E*)-*form* [760-82-7]
Fluoromaleic acid
Cryst. (Me_2CO/C_6H_6). Mp 132-133°.
Anhydride: [2714-23-0]. *3-Fluoro-2,5-furandione, 9CI.*
Fluoromaleic anhydride
C_4HFO_3 M 116.048
Bp 162°. n_D^{25} 1.4452.
(*Z*)-*form* [672-18-4]
Fluorofumaric acid
Cryst. (Et_2O/pet. ether). Mp 206-208° dec., Mp 236-237°.

Raasch, M. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 2678 (*anhydride*)
Akhtar, M. *et al*, *Tetrahedron*, 1987, **43**, 5899 (*synth, ir, pmr, cmr, ms*)

1-Fluorocyclohexanecarboxylic acid F-80031

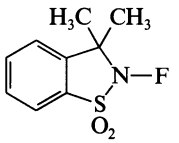
[117169-31-0]



$C_7H_{11}FO_2$ M 146.161
Oily solid.
Me ester: [117169-32-1].
$C_8H_{13}FO_2$ M 160.188
Oil.

Mongelli, N. *et al*, *Synthesis*, 1988, 310 (*synth, ir, pmr, cmr*)

N-Fluoro-2,3-dihydro-3,3-dimethyl-1,2-benzothiadiazole 1,1-dioxide F-80032



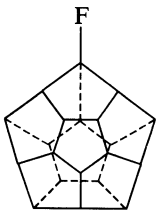
$C_9H_{10}FNO_2S$ M 215.248
Superior fluorinating agent for synth. of α-fluorocarbonyl compds. Cryst. Mp 114-116°.

Differding, E. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1248 (*synth, pmr, cmr, ms, use*)

Fluorododecahedrane F-80033

*1-Fluorohexadecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene, 9CI*

[112896-29-4]



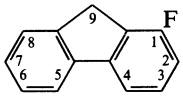
$C_{20}H_{19}F$ M 278.368

Solid. Mp >260°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **101**, 1303 (*synth, cmr*)

1-Fluoro-9*H*-fluorene F-80034

[343-25-9]



$C_{13}H_9F$ M 184.212
Cryst. (EtOH aq.). Mp 83-84°.

Suzuki, K. *et al*, *J. Org. Chem.*, 1959, **24**, 1511 (*synth, ir*)
Sardella, D.J. *et al*, *J. Fluorine Chem.*, 1984, **24**, 249.

2-Fluoro-9*H*-fluorene F-80035

[343-43-1]

$C_{13}H_9F$ M 184.212
Cryst. (C_6H_6). Mp 101-102°. pK_a 21.0 (DMSO,25°).

Bergmann, E.D. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 6037 (*synth*)
Fletcher, T.L. *et al*, *Chem. Ind.* (*London*), 1961, 179 (*synth*)
Bordwell, F.G. *et al*, *J. Org. Chem.*, 1976, **41**, 2391; 1988, **53**, 780 (*props*)
Kitching, W. *et al*, *Org. Magn. Reson.*, 1980, **14**, 502 (*cmr*)

3-Fluoro-9*H*-fluorene F-80036

[343-40-8]

$C_{13}H_9F$ M 184.212
Cryst. (cyclohexane). Mp 80°. pK_a 22.07 (DMSO, 25°C).

Suzuki, K. *et al*, *J. Org. Chem.*, 1959, **24**, 1511; 1961, **26**, 2236 (*synth*)
Bordwell, F.G. *et al*, *J. Org. Chem.*, 1988, **53**, 780 (*props*)

4-Fluoro-9*H*-fluorene F-80037

[317-71-5]

$C_{13}H_9F$ M 184.212
Cryst. (cyclopentane). Mp 38-39°.

Fletcher, T.L. *et al*, *J. Org. Chem.*, 1960, **25**, 996 (*synth*)
Buckle, D.R. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1979, 3004 (*synth*)

9-Fluoro-9*H*-fluorene F-80038

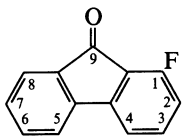
[20825-90-5]

$C_{13}H_9F$ M 184.212
Cryst. (MeOH at −60°). Mp 60-60.5°. Polymerises with loss of HF at r.t.

Streitwieser, A. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 2444 (*synth, uv, ir, pmr*)
Johnson, A.L., *J. Org. Chem.*, 1982, **47**, 5220 (*F nmr*)

1-Fluoro-9*H*-fluoren-9-one, 9CI F-80039

[1514-16-5]



$C_{13}H_7FO$ M 198.196
Cryst. (pet. ether or EtOH). Mp 110-111.5°.

Fletcher, T.L. *et al*, *J. Org. Chem.*, 1960, **25**, 996 (*synth*)
Fletcher, T.L. *et al*, *Chem. Ind.* (*London*), 1961, 179 (*synth*)
Agranat, I. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 7068 (*synth, F nmr*)

2-Fluoro-9*H*-fluoren-9-one F-80040

[343-01-1]

$C_{13}H_7FO$ M 198.196
Cryst. (MeOH). Mp 117-118°. Bp_{10} 185°.

Bergmann, E. *et al*, *Chem. Ber.*, 1933, **66**, 46 (*synth, deriv*)
Fletcher, T.L. *et al*, *Chem. Ind.* (*London*), 1961, 179 (*synth*)
Schaefer, T. *et al*, *Can. J. Chem.*, 1986, **64**, 2162 (*cmr, F nmr*)

3-Fluoro-9*H*-fluoren-9-one F-80041

[1514-15-4]

$C_{13}H_7FO$ M 198.196
Yellow needles (C_6H_6/pet. ether). Mp 129-130°.

Suzuki, K. *et al*, *J. Org. Chem.*, 1961, **26**, 2239 (*synth, uv*)
Dewar, M.J.S. *et al*, *J. Org. Chem.*, 1963, **28**, 1759 (*synth*)
Agranat, I. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 7068 (*F nmr*)

4-Fluoro-9*H*-fluoren-9-one F-80042

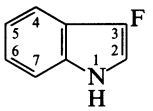
[1514-18-7]

$C_{13}H_7FO$ M 198.196
Yellow needles (EtOH). Mp 161-162.5°.

Fletcher, T.L. *et al*, *J. Org. Chem.*, 1960, **25**, 996 (*synth*)
Fletcher, T.L. *et al*, *Chem. Ind.* (*London*), 1961, 179 (*synth*)

3-Fluoro-1*H*-indole, 9CI F-80043

[66946-81-4]



C_8H_6FN M 135.140
Cryst. or liq. Mp ~20°.

Barton, D.H.R. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1977, 2604 (*synth, uv, ir, pmr*)
Ermolenko, M.S. *et al*, *Khim. Geterotsikl. Soedin.*, 1978, 933; *CA*, **89**, 146707v (*synth*)

4-Fluoro-1*H*-indole, 9CI F-80044

[387-43-9]

C_8H_6FN M 135.140
Prisms (MeOH aq.). Mp 29-30°. pK_a 16.30.
Picrate: Orange-red cryst. (C_6H_6). Mp 164-166°.
1,3,5-Trinitrobenzene complex: Orange-yellow cryst. (EtOH). Mp 172°.

Allen, F.L. *et al*, *J. Chem. Soc.*, 1955, 1283 (*synth, uv, derivs*)
Bentov, N. *et al*, *Isr. J. Chem.*, 1964, **2**, 25 (*synth*)
Yagil, G., *Tetrahedron*, 1967, **23**, 2855 (*props*)
Asher, K. *et al*, *Isr. J. Chem.*, 1968, **6**, 927.
Sugasawa, T. *et al*, *J. Org. Chem.*, 1979, **44**, 578 (*synth, ir*)
Somei, M. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 3696 (*synth, ir, pmr*)

5-Fluoro-1*H*-indole, 9CI F-80045

[399-52-0]

C_8H_6FN M 135.140
Cryst. (C_6H_6). Mp 46-47°. pK_a 16.30.
Picrate: Orange cryst. (C_6H_6). Mp 155-156°.

Allen, F.L. *et al*, *J. Chem. Soc.*, 1955, 1283 (*synth, uv, derivs*)
Pelchowicz, Z. *et al*, *J. Chem. Soc.*, 1961, 5418 (*synth*)
Hoffmann, E. *et al*, *J. Heterocycl. Chem.*, 1965, **2**, 298 (*synth*)
Yagil, G., *Tetrahedron*, 1967, **23**, 2855 (*props*)
Lallemand, J.Y. *et al*, *Bull. Soc. Chim. Fr.*, 1970, **11**, 4091 (*pmr*)
Sirowe, H. *et al*, *Synthesis*, 1972, 84 (*synth*)

Rosenberg, E. *et al*, *Org. Magn. Reson.*, 1976, **8**, 117 (*N*-15 *nmr*, *cmr*)
Ayachit, N.H. *et al*, *Spectrochim. Acta*, *Part A*, 1986, **42**, 781 (*ir*, *uv*)

6-Fluoro-1*H*-indole, 9CI F-80046

[399-51-9]
C_8H_6FN M 135.140
Cryst. (Et_2O/pet. ether). Mp 75-76°.
Picrate: Orange-red cryst. (C_6H_6). Mp 147-148°.

Allen, F.L. *et al*, *J. Chem. Soc.*, 1955, 1283, 1286 (*synth*, *uv*, *derivs*)
Bergmann, E.D. *et al*, *J. Chem. Soc.*, 1959, 1913 (*synth*)
Bentov, M. *et al*, *J. Chem. Soc.*, 1962, 2825 (*synth*)
Sugasawa, T. *et al*, *J. Org. Chem.*, 1979, **44**, 478 (*synth*)
Guo, W. *et al*, *Magn. Reson. Chem.*, 1986, **24**, 75 (*F*-19 *nmr*, *cmr*)
Ayachit, N.H. *et al*, *Spectrochim. Acta*, *Part A*, 1986, **42**, 781 (*uv*, *ir*)

7-Fluoro-1*H*-indole, 9CI F-80047

C_8H_6FN M 135.140
Cryst. (EtOH aq.). Mp 61-62°.
Picrate: Orange-red cryst. (C_6H_6). Mp 154-155°.

Allen, F.L. *et al*, *J. Chem. Soc.*, 1955, 1283 (*synth*, *uv*)

2-Fluoro-3-iodopyridine F-80048

[113975-22-7]

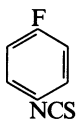
C_5H_3FIN M 222.988
Cryst. Mp 42°. Bp_{17} 97-99°.

Estel, L. *et al*, *J. Org. Chem.*, 1988, **53**, 2740 (*synth*, *ir*, *pmr*)

1-Fluoro-4-isothiocyanatobenzene, 9CI F-80049

p-*Fluorophenyl isothiocyanate*, *8CI*. *4-Fluorophenyl thiocarbimide*

[1544-68-9]

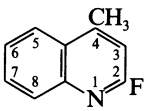


C_7H_4FNS M 153.180
Has fungicidal props. Oil. Mp 23.5-25.5° (12°). Bp 228°, $Bp_{1.3}$ 60°. n_D^{25} 1.6178.

Craig, C. *et al*, *Aust. J. Chem.*, 1960, **13**, 341 (*synth*)
Ham, N.S. *et al*, *Spectrochim. Acta*, *Part A*, 1960, **16**, 279 (*ir*)
Kinoshita, Y. *et al*, *Agric. Biol. Chem.*, 1966, **30**, 447 (*synth*)
Weigert, F.J. *et al*, *J. Org. Chem.*, 1976, **41**, 4006 (*F-nmr*)

2-Fluoro-4-methylquinoline, 9CI F-80050

2-Fluorolepidine, *8CI*



$C_{10}H_8FN$ M 161.178
Liq. Bp_{16} 140°.

U.K. Pat., 845 062, (1960); *CA*, **55**, 5544 (*synth*)

3-Fluoro-4-methylquinoline, 9CI F-80051

3-Fluorolepidine, *8CI*

[72473-78-0]
$C_{10}H_8FN$ M 161.178
Oil.

Dehmlow, E.V. *et al*, *Justus Liebigs Ann. Chem.*, 1979, 1456 (*synth*, *pmr*, *F nmr*)

4-Fluoro-2-methylquinoline, 9CI F-80052

4-Fluoroquinaldine, *8CI*

$C_{10}H_8FN$ M 161.178
Cryst. Mp 40° (hydrate). Bp_{16} 114°.

U.K. Pat., 845 062, (1960); *CA*, **55**, 5544 (*synth*)
Bellas, M. *et al*, *J. Chem. Soc.*, 1965, 2096 (*synth*)

6-Fluoro-2-methylquinoline, 9CI F-80053

6-Fluoroquinaldine, *8CI*

[1128-61-6]
$C_{10}H_8FN$ M 161.178
Cryst. (Et_2O/hexane). Mp 57-59°.

Leir, C.M., *J. Org. Chem.*, 1977, **42**, 911 (*synth*)

6-Fluoro-5-methylquinoline, 9CI F-80054

[107224-22-6]
$C_{10}H_8FN$ M 161.178
Oil.

Gerster, J.F. *et al*, *J. Med. Chem.*, 1987, **30**, 839 (*synth*)

7-Fluoro-2-methylquinoline, 9CI F-80055

7-Fluoroquinaldine, *8CI*

[1128-74-1]
$C_{10}H_8FN$ M 161.178
Bp_{15} 120°.
Hydrate: Mp 38°.
B,HNO$_3$: Mp 137° dec.

Haigh, C.W., *J. Chem. Soc.*, 1965, 6004 (*synth*, *pmr*)

2-Fluorooctadecanoic acid F-80056

2-Fluorostearic acid

[1578-61-6]

$H_3C(CH_2)_{15}CHFCOOH$

$C_{18}H_{35}FO_2$ M 302.472
(±)-*form*
Cryst. Mp 88-90°.
Me ester:
$C_{19}H_{37}FO_2$ M 316.498
Cryst. (MeOH). Mp 42-44°.

Pattison, F.L. *et al*, *Can. J. Chem.*, 1965, **43**, 1700 (*synth*)
Pogány, S.A. *et al*, *Synthesis*, 1987, 718 (*synth*, *ir*, *pmr*, *cmr*, *F nmr*)

18-Fluoro-9-octadecenoic acid F-80057

ω-Fluorooleic acid

$FCH_2(CH_2)_7CH{=}CH(CH_2)_7COOH$

$C_{18}H_{33}FO_2$ M 300.456
(*Z*)-*form*
Isol. from seeds of *Dichapetalum toxicarium*. Oil or cryst. Mp 13.5°.

Peters, R.A. *et al*, *Biochem. J.*, 1960, **71**, 17 (*isol*)
Dean, R.E.A. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 612 (*synth*)

1-Fluorooctane, 9CI F-80058

[463-11-6]

$H_3C(CH_2)_6CH_2F$

$C_8H_{17}F$ M 132.221
Liq. d 0.81. Bp 142-144°. n_D^{20} 1.3955.

Macey, W.A.T., *J. Phys. Chem.*, 1960, **64**, 254 (*synth*)
Landini, D. *et al*, *Synthesis*, 1974, 428 (*synth*)
Badone, D. *et al*, *Synthesis*, 1987, 920 (*synth*)

1-Fluoro-2-phenylethane F-80059

(2-Fluoroethyl)benzene, 9CI

[458-87-7]

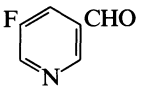
$PhCH_2CH_2F$

C_8H_9F M 124.157
Liq. Bp_{10} 53-54°.

DePuy, C.H. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 2535 (*synth*)
Koch, M.F. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 5423 (*synth, pmr*)
Badone, D. *et al*, *Synthesis*, 1987, 920 (*synth, pmr*)

5-Fluoro-3-pyridinecarboxaldehyde F-80060

[39891-04-8]



C_6H_4FNO M 125.102
Liq. Bp_{22} 90°, Bp_{10} 71-76°.

Kyba, E.P. *et al*, *J. Org. Chem.*, 1988, **53**, 3513 (*synth, pmr, F nmr, ir*)

5-Fluoropyrimidine, 9CI F-80061

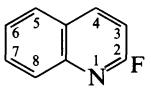
[675-21-8]

$C_4H_3FN_2$ M 98.079
Bp_{733} 101-102°. n_D^{19} 1.4693.

Reichardt, C. *et al*, *Justus Liebigs Ann. Chem.*, 1975, 470 (*synth, F nmr, pmr*)

2-Fluoroquinoline, 9CI F-80062

[580-21-2]



C_9H_6FN M 147.151
Bp_{30} 130-133°, Bp_2 75°. n_D^{25} 1.5827.

B,HNO$_3$: Cryst. (EtOH). Mp 137-141°.

Picrate: Mp 227-229°.

N-*oxide:*
C_9H_6FNO M 163.151
Mp 67°.

Roe, A. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 1785 (*synth*)
Miller, W.K. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 1629 (*uv*)
Hamer, J. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1962, **81**, 1058 (*synth*)
Dewar, M.J.S. *et al*, *J. Chem. Phys.*, 1968, **49**, 499 (*F nmr*)

3-Fluoroquinoline, 9CI F-80063

[396-31-6]

C_9H_6FN M 147.151
d_4^{25} 1.19. Bp_{15} 102°. n_D^{25} 1.5902. Nonmutagenic. Forms solid hydrate.

Picrate: [448-47-5].
Mp 185-186° (183-185°).

N-*oxide:*
C_9H_6FNO M 163.151
Mp 118°.

N-*oxide, picrate:* Cryst. (EtOH). Mp 130°.

Roe, A. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 1785 (*synth*)
Miller, W.K. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 1629 (*uv*)
Bellas, M. *et al*, *J. Chem. Soc.*, 1963, 4007 (*oxide*)
Dewar, M.J.S. *et al*, *J. Chem. Phys.*, 1968, **49**, 499 (*F nmr*)
Doddrell, D. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1976, 402 (*cmr*)
Takahashi, K. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4630 (*tox*)

4-Fluoroquinoline, 9CI F-80064

[394-70-7]

C_9H_6FN M 147.151
Synth. not certain. Bp_{30} 119° (?) .

Roe, A. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 1785 (*synth*)

5-Fluoroquinoline, 9CI F-80065

[394-69-4]

C_9H_6FN M 147.151
d_4^{25} 1.19. Bp_{30} 123°, Bp_{15} 107-108°. n_D^{25} 1.5916.

▷ Mutagenic.

Picrate: Mp 199-200.5°.

N-*oxide:*
C_9H_6FNO M 163.151
Mp 176°.

N-*oxide, picrate:* Mp 136°.

Roe, A. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 1785 (*synth*)
Miller, W.K. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 1629 (*uv*)
Palmer, M.H., *J. Chem. Soc.*, 1962, 3645 (*synth*)
Bellas, M. *et al*, *J. Chem. Soc.*, 1963, 4007 (*oxide*)
Haigh, C.W. *et al*, *J. Chem. Soc.*, 1965, 6004 (*pmr*)
Dewar, M.J.S. *et al*, *J. Chem. Phys.*, 1968, **49**, 499 (*F nmr*)
Doddrell, D. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1976, 402 (*cmr*)
Takahashi, K. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4630 (*tox*)

6-Fluoroquinoline, 9CI F-80066

[396-30-5]

C_9H_6FN M 147.151
d_4^{25} 1.20. Bp_{30} 124-126°. n_D^{25} 1.5908. Forms solid hydrate.

▷ Weakly mutagenic.

Picrate: Mp 218-219°.

N-*oxide:* [2338-74-1].
C_9H_6FNO M 163.151
Mp 100°.

N-*oxide, picrate:* Mp 130°.

Roe, A. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 1785 (*synth*)
Miller, W.K. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 1629 (*uv*)
Sveinbjornsson, A. *et al*, *J. Org. Chem.*, 1951, **16**, 1450 (*synth*)
Bellas, M. *et al*, *J. Chem. Soc.*, 1963, 4007 (*oxide*)
Dewar, M.J.S. *et al*, *J. Chem. Phys.*, 1968, **49**, 499 (*F nmr*)
Doddrell, D. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1976, 402 (*C-13 nmr*)
Takahashi, K. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4630 (*tox*)

7-Fluoroquinoline, 9CI F-80067

[396-32-7]

C_9H_6FN M 147.151

Shows herbicidal props. Bp_{15} 107-108° (112°) . n_D^{25} 1.5845. n_D^{20} 1.5915.

Roe, A. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 1785 (*synth*)
Miller, W.K. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 1629 (*uv*)
Palmer, M.H., *J. Chem. Soc.*, 1962, 3645 (*synth*)
Bellas, M. *et al*, *J. Chem. Soc.*, 1963, 4007 (*oxide*)
Haigh, C.W. *et al*, *J. Chem. Soc.*, 1965, 6004 (*pmr*)
Dewar, M.J.S. *et al*, *J. Chem. Phys.*, 1968, **49**, 499 (*F nmr*)

8-Fluoroquinoline, 9CI F-80068

[394-68-3]

C_9H_6FN M 147.151

d_4^{25} 1.21. Bp_{30} 148-150°. n_D^{25} 1.6028.

▷ Mutagenic.

Picrate: [394-62-7].
Mp 170-172°.

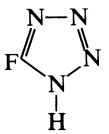
N-*oxide:* [2795-43-9].
C_9H_6FNO M 163.151
Hygroscopic solid. Mp 64°.

N-*oxide, picrate:* Cryst. (EtOH). Mp 128°.

Roe, A. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 1785 (*synth*)
Miller, W.K. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 1629 (*uv*)
Bellas, M. *et al*, *J. Chem. Soc.*, 1963, 4007 (*oxide*)
Dewar, M.J.S. *et al*, *J. Chem. Phys.*, 1968, **49**, 499 (*F nmr*)
Doddrell, D. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 2, 1976, 402 (*cmr*)
Sibi, M.P. *et al*, *Org. Magn. Reson.*, 1980, **14**, 494 (*N*-15 *nmr*)
Takahashi, K. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4630 (*tox*)

5-Fluoro-1*H*-tetrazole, 9CI, 8CI F-80069

[60471-49-0]



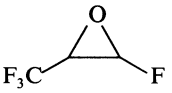
$CHFN_4$ M 88.044

1-Benzyl:
$C_8H_7FN_4$ M 178.168
Yellow oil.

U.S. Pat., 530 260, (1974); *CA*, **85**, 102223 (*synth*)
Klich, M. *et al*, *Tetrahedron*, 1986, **42**, 2677 (*deriv*, *synth*, *ir*, *pmr*)

2-Fluoro-3-(trifluoromethyl)oxirane F-80070

2,3-Epoxy-1,1,1,3-tetrafluoropropane, 8CI. 1,3,3,3-Tetrafluropropylene oxide



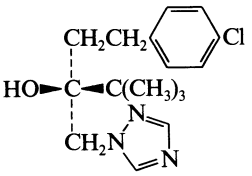
$C_3H_2F_4O$ M 130.042

Bp 37°. Prob. mixt. of stereoisomers.

McBee, E.T. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 4091 (*synth*)

Folicur F-80071

*α-[2-(4-Chlorophenyl)ethyl]-α-(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol, 9CI. Raxil. HWG-1608*



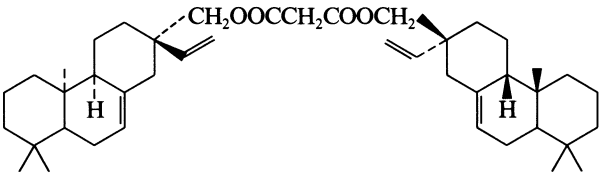
$C_{16}H_{22}ClN_3O$ M 307.822

(*S*)-*form* [119364-85-1]
Fungicide functioning as ergosterol-biosynthesis inhibitor. $[\alpha]_D^{20}$ −34.0° (c, 1 in $CHCl_3$). This is the more active enantiomer.

[107534-96-3]

Kaulen, J., *Angew. Chem.*, *Int. Ed. Engl.*, 1989, **28**, 462 (*synth*, *abs config*, *bibl*)

Foliosate F-80072



$C_{43}H_{64}O_4$ M 644.976

Constit. of *Calceolaria foliosa*. Gum. $[\alpha]_D^{25}$ −133.7° (c, 1.07 in $CHCl_3$).

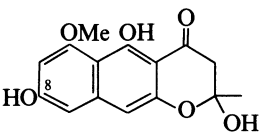
Chamy, M.C. *et al*, *Phytochemistry*, 1989, **28**, 571.

Fonsecin F-80073

Updated Entry replacing F-00654

*2,3-Dihydro-2,5,8-trihydroxy-6-methoxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, 9CI*

[3748-39-8]



$C_{15}H_{14}O_6$ M 290.272

Pigment from a mutant of *Aspergillus fonsecaeus* and *A. carbonarius*. Mycotoxin. Bright-yellow irregular prisms. Mp 198° dec. λ_{max} 233 (log ε 4.42), 275(4.50), 321 (3.86), 332 (3.90) and 400 nm (3.94).

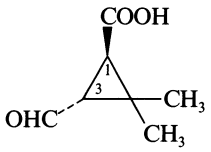
O^8-*Me:* [1856-95-7]. ***Fonsecin B***
$C_{16}H_{16}O_6$ M 304.299
Metab. of *A. fonsecaeus* and *A. niger*. Yellow needles (Me_2CO aq.). Mp 176°. Dehydration gives Rubrofusarin B.

Raper, K.B., *J. Elisha Mitchell Sci. Soc.*, 1953, **69**, 1 (*isol*)
Galmanini, O.L. *et al*, *Nature* (*London*), 1962, **195**, 502 (*isol*)
Galmanini, O.L. *et al*, *Experientia*, 1974, **30**, 586 (*deriv*)
Ehrlich, K.C. *et al*, *Appl. Environ. Microbiol.*, 1984, **48**, 1 (*deriv*)
Bloomer, J.L. *et al*, *J. Org. Chem.*, 1984, **49**, 5027 (*isol*, *cmr*, *biosynth*)
Priestap, H.A., *Tetrahedron*, 1984, **40**, 3617 (*pmr*)

3-Formyl-2,2-dimethyl-1-cyclopropane-carboxylic acid F-80074

Caronaldehydic acid

[25312-79-2]



(1*R*,3*R*)-*form*

$C_7H_{10}O_3$ M 142.154

Intermed. for synth. of pyrethroids.

(1R,3R)-form [31062-21-2]

Me ester: [27335-33-7].

$C_8H_{12}O_3$ M 156.181

Gum. $[\alpha]_D^{19}$ +19.3° (c, 0.38 in Me_2CO), $[\alpha]_D^{22}$ +15.3° (c, 12 in $CHCl_3$).

(1S,3S)-form [26883-41-0]

Me ester: [26770-99-0].

$[\alpha]_D$ −0.45° (c, 2.93 in $CHCl_3$).

(1R,3S)-form [28075-68-5]

Me ester: [55701-02-5].

$[\alpha]_D^{22}$ −72°, $[\alpha]_D^{25}$ −23.1° (c, 3.2 in $CHCl_3$).

(1S,3R)-form [40556-99-8]

Me ester: [84710-48-5].

$[\alpha]_D^{20}$ +79.8° (c, 0.18 in Me_2CO).

(1RS,3RS)-form [54984-59-7]

(±)-trans-*form*

Cryst. (EtOAc/hexane). Mp 80.5°.

2,4-Dinitrophenylhydrazone: Cryst. (EtOH-EtOAc). Mp 206°, Mp 208°.

Me ester: [41301-44-4].

Oil. $Bp_{0.75}$ 47-49°.

(1RS,3SR)-form [56711-70-7]

(±)-*cis-form*

Prisms (hexane), plates (EtOAc/hexane). Mp 84-85° (79°). In equilib. with hemiacetal.

2,4-Dinitrophenylhydrazone: Orange-yellow prisms (EtOH/EtOAc). Mp 207-209° dec.

Me ester: [51424-62-5].

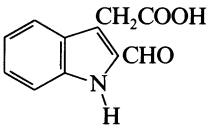
Pale yellow oil.

[27335-34-8, 54984-59-7, 67528-52-3, 67968-42-7]

Matsui, M. *et al*, *Agric. Biol. Chem.*, 1963, **27**, 554; 1964, **28**, 32 (*synth, deriv*)
Sugiyama, T. *et al*, *Agric. Biol. Chem.*, 1975, **39**, 1483 (*synth*)
Ortiz de Montellano, P.R. *et al*, *J. Org. Chem.*, 1978, **43**, 4323 (*synth*)
Devos, M.J. *et al*, *Tetrahedron Lett.*, 1978, 1847 (*synth, deriv*)
Crombie, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1711 (*synth, ir, pmr, ester*)
Martel, J.J. *et al*, *Pestic. Sci.*, 1980, **11**, 188 (*synth, resoln*)
Jakovuc, I.J. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 4659 (*synth, deriv*)
Gupta, D. *et al*, *Tetrahedron*, 1982, **38**, 3013 (*synth, pmr*)
Franck-Neumann, M. *et al*, *Tetrahedron Lett.*, 1982, **23**, 3493 (*synth, deriv*)
Tessier, J., *Chem. Ind.* (*London*), 1984, 199 (*manuf, resoln*)
Matsuo, A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1984, 203 (*synth, ir, pmr, deriv*)
Takano, S. *et al*, *Heterocycles*, 1985, **23**, 2859 (*synth, deriv*)
Frauenrath, H. *et al*, *Justus Liebigs Ann. Chem.*, 1985, 1303 (*synth, ir, pmr, deriv*)
Mujiani, Z. *et al*, *Synth. Commun.*, 1988, **18**, 135 (*synth, ir, pmr*)

2-Formyl-1*H*-indole-3-acetic acid, 9CI F-80075

[118361-82-3]



$C_{11}H_9NO_3$ M 203.197

Pale yellow solid. Mp 197-200°.

Et ester: [118361-81-2].

$C_{13}H_{13}NO_3$ M 231.251

Mp 79-80°.

Moody, C.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1407 (*synth, ir, pmr, ms*)

Formylmethanesulfonic acid F-80076

$OHCCH_2SO_3H$

$C_2H_4O_4S$ M 124.117

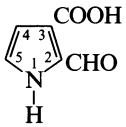
Esters prepd. and used as Li enolates and characterised as dinitrophenylhydrazones.

[120263-38-9, 120263-39-0, 120263-42-5]

Berkessel, A. *et al*, *Chem. Ber.*, 1989, **122**, 1147.

2-Formyl-1*H*-pyrrole-3-carboxylic acid F-80077

[51361-92-3]



$C_6H_5NO_3$ M 139.110

Cryst. (H_2O). Mp 245°.

Me ester: [19075-68-4].

$C_7H_7NO_3$ M 153.137

Needles (H_2O). Mp 129°.

Et ester: [19076-57-4].

$C_8H_9NO_3$ M 167.164

Cryst. (C_6H_6/hexane). Mp 120° (117.5°).

Bisagni, E. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 637 (*synth*)
Farnier, M. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2335 (*synth, pmr*)

4-Formyl-1*H*-pyrrole-2-carboxylic acid F-80078

$C_6H_5NO_3$ M 139.110

Cryst. (H_2O). Mp 220°.

Et ester: [7126-57-0].

$C_8H_9NO_3$ M 167.164

Cryst. (pet. ether). Mp 104-106°. $Bp_{0.1}$ 115-136°.

Khan, M.K.A. *et al*, *Tetrahedron*, 1966, **22**, 2095 (*synth, ir, pmr*)

5-Formyl-1*H*-pyrrole-2-carboxylic acid F-80079

[7126-51-4]

$C_6H_5NO_3$ M 139.110

Prod. in cultures of *Erwinia oxoidiae*. Cryst. (H_2O). Mp 202-203° (212-215° dec.).

Me ester: [1197-13-3].

$C_7H_7NO_3$ M 153.137

Cryst. (pet. ether). Mp 92-93°.

Et ester: [7126-50-3].

$C_8H_9NO_3$ M 167.164

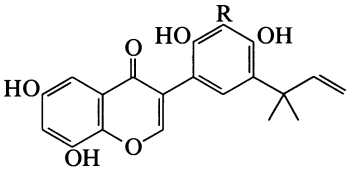
Cryst. (pet. ether). Mp 75°. $Bp_{0.1}$ 96-100°.

1-Me, Me ester:

$C_8H_9NO_3$ M 167.164
Cryst. (pet. ether). Mp 100-102°.

Reichstein, T., *Helv. Chim. Acta*, 1930, **13**, 349 (*synth*)
Khan, M.K.A. *et al*, *Tetrahedron*, 1966, **22**, 2095 (*synth, ir, pmr*)

Fremontin F-80080



R = H

$C_{20}H_{18}O_6$ M 354.359
Constit. of *Psorothamnus fremontii*. Cryst. Mp 244-247°.

Manikumar, G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 769 (*isol, pmr, cmr*)

Fremontone F-80081

As Fremontin, F-80080 with

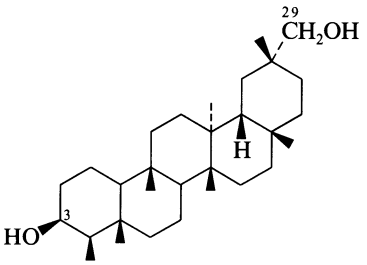
R = $-CH_2CH{=}C(CH_3)_2$

$C_{25}H_{26}O_6$ M 422.477
Constit. of *Psorothamnus fremontii*. Cryst. Mp 124-126°.

Manikumar, G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 769 (*isol, pmr, cmr*)

3,29-Friedelanediol F-80082

D:A-Friedooleanane-3,29-diol, 9CI



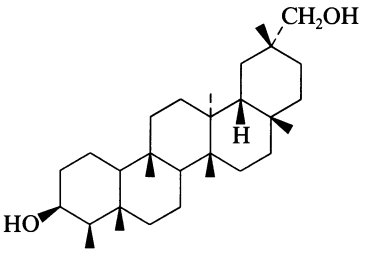
$C_{30}H_{52}O_2$ M 444.740

3β-form
Constit. of *Mortonia palmerii*. Cryst. Mp 270-272°.

3-Ketone, 29-aldehyde: [39903-23-6]. *3-Oxo-29-friedelanal*
$C_{30}H_{48}O_2$ M 440.708
Constit. of *M. diffusa*. Cryst. Mp 273-275°.

Domínguez, X.A. *et al*, *Phytochemistry*, 1974, **13**, 1292 (*isol*)
Martínez, V.M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 793 (*struct*)

3,30-Friedelanediol F-80083



$C_{30}H_{52}O_2$ M 444.740

3β-form
Needles ($CHCl_3$/MeOH). Mp 294-296°. $[\alpha]_D^{30}$ +13.9° (c, 1 in $CHCl_3$).

3-Ac: 3β-Acetoxy-30-friedelanol
$C_{32}H_{54}O_3$ M 486.777
Constit. of *Euphorbia antiquorum*. Plates ($CHCl_3$/MeOH). Mp 311-312°. $[\alpha]_D^{30}$ +62.8° (c, 0.8 in $CHCl_3$).

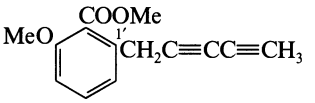
30-Ac: 30-Acetoxy-3β-friedelanol
$C_{32}H_{54}O_3$ M 486.777
Constit. of *E. antiquorum*. Plates ($CHCl_3$/MeOH). Mp 238-240°. $[\alpha]_D^{30}$ +27.5° (c, 0.8 in $CHCl_3$).

Di-Ac: 3β,30-Diacetoxyfriedelane
$C_{34}H_{56}O_4$ M 528.814
Constit. of *E. antiquorum*. Plates ($CHCl_3$/MeOH). Mp 268-269°. $[\alpha]_D^{30}$ +23.5° (c, 0.85 in $CHCl_3$).

Anjaneyulu, V. *et al*, *Phytochemistry*, 1989, **28**, 1695.

Frutescin† F-80084

Methyl 2-(2,4-hexadiynyl)-6-methoxybenzoate, 9CI
[4368-08-5]



$C_{15}H_{14}O_3$ M 242.274
Isol. from roots of *Chrysanthmum frutescens* and *C. foeniculatum*. Cryst. (pet. ether). Mp 69°. (pet. ether). Mp 69°.

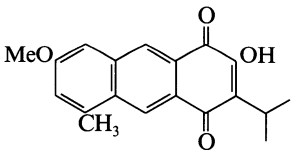
1′-Acetoxy: ***Fruscinol acetate***
$C_{17}H_{16}O_5$ M 300.310
Isol. from *C. frutescens* and *C. foeniculatum*. Cryst. (Et_2O/pet. ether). $[\alpha]_D^{20}$ −10° (c, 1.9 in Et_2O).

1′-Oxo: ***Frutescinone***
$C_{15}H_{12}O_4$ M 256.257
Isol. from roots of *C. frutescens*. Yellowish cryst. (Et_2O). Mp 121°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 602; 1964, **97**, 1176, 1179; 1966, **99**, 995, 2822 (*isol, uv, ir, struct, synth, biosynth*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1969, **102**, 3298 (*synth*)

Fruticulin B F-80085

Updated Entry replacing F-60077
[106664-41-9]



$C_{19}H_{18}O_6$ M 342.348
Constit. of *Salvia fruticulosa*. Cryst. (Me_2CO). Mp 173-174°.

Rodriguez-Hahn, L. *et al*, *Phytochemistry*, 1989, **28**, 567 (*isol, cryst struct*)

Fulminic acid, 9CI, 8CI F-80086

Updated Entry replacing F-00777
Carbyloxime
[51060-05-0]

$HC{\equiv}N^{\oplus}{-}O^{\ominus}$

CHNO M 43.025

Shown to have the struct. shown rather than $C^{\ominus}\equiv N^{\oplus}OH$ which was prev. postulated. Metal salts are widely used in detonators. The free acid is stable for a time only in Et_2O sol. at low temps.; it polymerises rapidly.

▷ Salts highly explosive, shock-sensitive, Hg salt is highly toxic. LS9320000.

Trimolecular Me ester:
C_2H_3NO M 57.052
Needles (H_2O). Mp 149°.

[506-85-4]

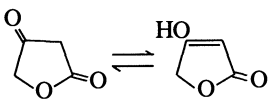
Wieland, H., *Ber.*, 1910, **43**, 3362 (*synth*)
Wöhler, L. *et al*, *Ber.*, 1929, **62**, 2742, 2748 (*salts*)
Beck, W. *et al*, *Chem. Ber.*, 1971, **104**, 533 (*ir, struct*)
Grundmann, C. *et al*, *Justus Liebigs Ann. Chem.*, 1973, 898 (*synth*)
Rodd's Chem. Carbon Compd. (*2nd Ed.*), 2nd Ed., 1973, 143 (*rev*)
De Sarlo, F. *et al*, *Tetrahedron*, 1985, **41**, 5181 (*synth, props*)
Teles, J.H. *et al*, *Chem. Ber.*, 1989, **122**, 753 (*struct, bibl*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 276, 405.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 696, 972.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society ofChemistry, London, 1981, 383, 471.

2,4-(3*H*,5*H*)-Furandione, 9CI F-80087

Updated Entry replacing F-00825

3,4-Dihydroxycrotonolactone. 3-Oxobutyrolactone. 4-Hydroxyacetoacetic lactone. Tetronic acid

[4971-56-6]



$C_4H_4O_3$ M 100.074
Plates (EtOH/ligroin). V. sol. H_2O. Mp 141°. Sinters at 135°. Strong monobasic acid.

Oxime:
$C_4H_5NO_3$ M 115.088
Plates (EtOH). Dec. at 146°.

Phenylhydrazone: Prisms (EtOH aq.). Mp 128°.

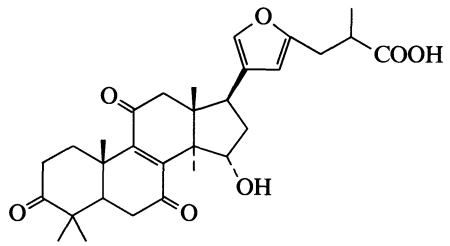
Me ether: [69556-70-3]. *4-Methoxy-2(5H)-furanone*
$C_5H_6O_3$ M 114.101
Cryst. Mp 66°.

Et ether: [69556-72-5]. *4-Ethoxy-2(5H)-furanone*
$C_6H_8O_3$ M 128.127
Faint yellow liq.

Mulholland, T.P.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 1225 (*synth*)
Greenhill, J.V. *et al*, *Tetrahedron Lett.*, 1974, 2683 (*synth*)
Tanaka, K. *et al*, *Chem. Pharm. Bull.*, 1979, **27**, 1901 (*synth*)
Schmidt, D.G. *et al*, *Synth. Commun.*, 1981, **11**, 385 (*synth*)
Grob Schmidt, D. *et al*, *J. Org. Chem.*, 1983, **48**, 1914 (*use, bibl*)
Zimmer, H. *et al*, *J. Org. Chem.*, 1988, **53**, 3368 (*ethers, synth, pmr, ir*)

Furanoganoderic acid F-80088

[120481-74-5]



$C_{30}H_{38}O_7$ M 510.626
Constit. of *Ganoderma applantum*. $[\alpha]_D^{23}$ +70° (c, 0.2 in EtOH).

Nishitoba, T. *et al*, *Phytochemistry*, 1989, **28**, 193.

2-Furanpropanal, 9CI F-80089

2-Furanpropionaldehyde, 8CI. 3-(2-Furyl)propanal. Furfurpropionaldehyde

[4543-51-5]

$C_7H_8O_2$ M 124.139
Liq. d_{19}^{19} 1.06. Bp_{17} 81°, Bp_4 59-61°.

Semicarbazone: Mp 82-83°.

Di-Me acetal: 2-(3,3-Dimethoxypropyl)furan
$C_9H_{14}O_3$ M 170.208
Liq. d_{20} 1.03. Bp_4 77°.

Weinhaus, H. *et al*, *CA*, 1930, **24**, 2127 (*synth*)
Sherlin, S.M. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1938, **8**, 7 (*synth*)

3-Furanpropanal, 9CI F-80090

3-(3-Furyl)propionaldehyde

[56859-93-9]

$C_7H_8O_2$ M 124.139
Liq. Bp_{10} 90-95°.

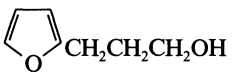
2,4-Dinitrophenylhydrazone: [56859-95-1]. Mp 118°.

Vig, O.P. *et al*, *J. Indian Chem. Soc.*, 1975, **52**, 199 (*synth, ir*)

2-Furanpropanol, 9CI F-80091

3-(2-Furyl)-1-propanol

[26908-23-6]



$C_7H_{10}O_2$ M 126.155
Oil. d_{20} 1.03. Bp_6 92-94°, $Bp_{0.2}$ 43-44°.

Bel'skii, I.F. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1964, 326 (*synth*)
DeShong, P. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1901 (*synth, ir, pmr*)

3-Furanpropanol, 9CI F-80092

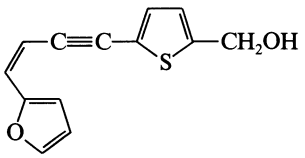
3-(3-Furyl)-1-propanol

[56859-92-8]

$C_7H_{10}O_2$ M 126.155
Liq. Bp_8 115-120°.

Vig, O.P. *et al*, *J. Indian Chem. Soc.*, 1975, **52**, 199 (*synth, ir*)

5-[4-(2-Furanyl)-3-buten-1-ynyl]-2-thiophenemethanol F-80093



$C_{13}H_{10}O_2S$ M 230.287

(Z)-form

Ac: ***1-(2-Furyl)-4-(5-acetoxymethyl-2-thienyl)-1-buten-3-yne***
$C_{15}H_{12}O_3S$ M 272.324
Isol. from *Santolina* sp. Cryst. (Et_2O/pet. ether). Mp 52.5-53°.

O-(*3-Methylbutanoyl*): [41628-63-1]. ***1-(2-Furyl)-4[5-(isovaleryloxymethyl)-2-thienyl]-1-buten-3-yne***
$C_{18}H_{18}O_3S$ M 314.404
Constit. of *S. rosmarinifolia*. Oil.

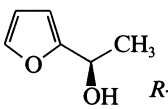
Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 135; 1973, **106**, 845 (*isol, uv, ir, pmr, struct*)

1-(2-Furanyl)ethanol F-80094

Updated Entry replacing H-01785

α-Methyl-2-furanmethanol, 9CI. Methyl-2-furylcarbinol. α-Methylfurfuryl alcohol. 2-(1-Hydroxyethyl)furan

[4208-64-4]



R-form

$C_6H_8O_2$ M 112.128

(R)-form
Bp_{15} 70°. $[\alpha]_D^{25}$ +19.09° (c, 1.10 in $CHCl_3$)(94% e.e.). n_D^{15} 1.4828.

Ac:
$C_8H_{10}O_3$ M 154.165
Bp_{11} 77°. n_D^{16} 1.4616.

(S)-form [27948-61-4]
Bp_{15} 70°. $[\alpha]_D^{25}$ −18.4° (c, 6 in EtOH)(89% e.e.). n_D^{15} 1.4827.

(±)-form
d_{25}^{25} 1.077. Bp 162-163°, Bp_{23} 76-77°. n_D^{15} 1.4827.

Ac: Bp_{760} 177°, Bp_{18} 85°. n_D^{25} 1.4618.

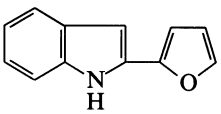
Acid phthalate: Mp 80°.

Peters, F.N. *et al*, *J. Am. Chem. Soc.*, 1930, **52**, 2081 (*synth*)
Duveen, D.I. *et al*, *J. Chem. Soc.*, 1936, 621 (*synth*)
Crombie, L. *et al*, *J. Solution Chem.*, 1950, 1707 (*synth*)
Pascal, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1965, 2211 (*pmr*)
Drueckhammer, D.G. *et al*, *J. Org. Chem.*, 1988, **53**, 1607 (*synth, resoln, pmr*)

2-(2-Furanyl)-1*H*-indole, 9CI F-80095

2-(2-Indolyl)furan

[54864-36-7]



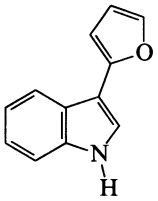
$C_{12}H_9NO$ M 183.209
Pale yellow flakes (C_6H_6/pet. ether). Mp 123-124°.

Calvaire, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1960, **250**, 3194 (*synth*)
Shivarama, H.B. *et al*, *Indian J. Chem., Sect. B*, 1976, **14**, 579 (*synth*)
Shivarama, H.B. *et al*, *Indian J. Chem., Sect. B*, 1979, **17**, 187 (*ms*)

3-(2-Furanyl)-1*H*-indole F-80096

2-(3-Indolyl)furan

[112616-94-1]



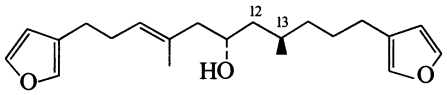
$C_{12}H_9NO$ M 183.209
Pale brown solid. Mp 90-91°.

Campbell, M.M. *et al*, *Tetrahedron*, 1987, **43**, 1117 (*synth, uv, ir, pmr, ms*)

Furospongin I F-80097

Updated Entry replacing F-00923

[35075-74-2]



$C_{21}H_{30}O_3$ M 330.466
Constit. of *Spongia officinalis* and *Hippospongia communis*. Cryst. (pet. ether). Mp 35°. $[\alpha]_D$ +8.8° (c, 1 in $CHCl_3$).

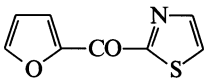
12,13-Didehydro: ***12,13-Didehydrofurospongin I***
$C_{21}H_{28}O_3$ M 328.450
Constit. of *Carteriospongia flabellifera*.

Cimino, G. *et al*, *Tetrahedron*, 1971, **27**, 4673 (*isol, struct*)
Schmitz, F.J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 745 (*deriv*)

2-Furyl 2-thiazolyl ketone F-80098

2-Furanyl 2-thiazolylmethanone. 2-(2-Furoyl)thiazole

[112969-91-2]



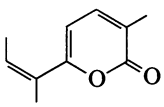
$C_8H_5NO_2S$ M 179.199
Oil.

Dondoni, A. *et al*, *J. Org. Chem.*, 1988, **53**, 1748 (*synth, ir, pmr*)

Fusalanipyrone F-80099

3-Methyl-6-(1-methyl-1-propenyl)-2H-pyran-2-one, 9CI

[118169-29-2]



$C_{10}H_{12}O_2$ M 164.204
Metab. of *Fusarium solani*. Oil.

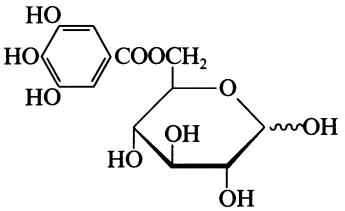
Abraham, W.-R. *et al*, *Phytochemistry*, 1988, **27**, 3310.

G

6-Galloylglucose G-80001

β-D-Glucopyranose 6-(3,4,5-trihydroxybenzoate), 9CI

[34781-46-9]



$C_{13}H_{16}O_{10}$ M 332.263

Isol. from rhizomes of *Geranium pratense* and *Polygonum bistorta*. Cryst. + $2H_2O$ (H_2O). Mp 166° (sinters from 110°). $[\alpha]_D$ +54.5° → +36.8° (12h) (c, 1.9 in H_2O).

[13186-19-1, 33040-89-0]

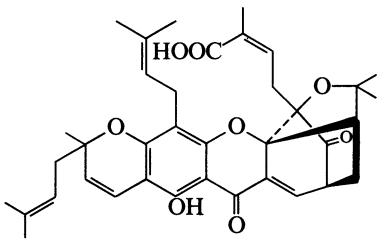
Schmidt, O.T. *et al*, *Justus Liebigs Ann. Chem.*, 1951, **571**, 29 (*synth*)

Gstirner, F. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1962, **295**, 23; 1966, **299**, 640 (*isol*)

Gambogic acid G-80002

Guttic acid. Guttatic acid

[2752-65-0]



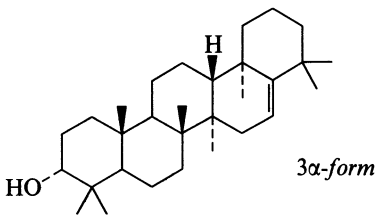
$C_{37}H_{42}O_8$ M 614.734

The name Guttic (Guttatic) acid is a transliteration of the French/Italian names for the substance. The English equiv. is stated to be Gambogic acid. Gamboge is also known as Gummi Gutta. Isol. from Gamboge resin.

Amorosa, M. *et al*, *Ann. Chim.* (*Rome*), 1966, **56**, 232.

Arnone, A. *et al*, *Tetrahedron Lett.*, 1967, 4201 (*pmr, struct*)

16-Gammaceren-3-ol G-80003



3α-*form*

$C_{30}H_{50}O$ M 426.724

3α-form

Constit. of *Picris hieracioides*. Cryst. Mp 269-270°. $[\alpha]_D^{23}$ +99° (c, 0.6 in $CHCl_3$).

3β-form

Constit. of roots of *P. hieracioides*. Cryst. Mp 254-256°. $[\alpha]_D^{23}$ +36.6° (c, 0.3 in $CHCl_3$).

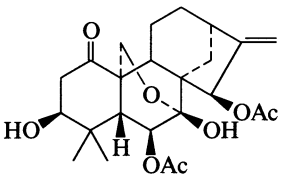
Ac:

$C_{32}H_{52}O_2$ M 468.762

Constit. of *P. hieracioides*. Mp 287-288°. $[\alpha]_D^{23}$ +36.0° (c, 0.5 in $CHCl_3$).

Shiojima, K. *et al*, *Tetrahedron Lett.*, 1989, **30**, 4977 (*cryst struct*)

Ganervosin A G-80004

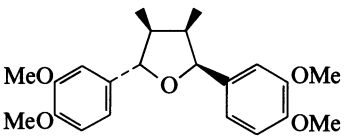


$C_{24}H_{32}O_8$ M 448.512

Constit. of *Rabdosia nervosa*. Cryst. (Me_2CO). Mp 224-226°.

Wang, Q.-G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 775 (*isol, cryst struct*)

Ganschisandrine G-80005



$C_{22}H_{28}O_5$ M 372.460

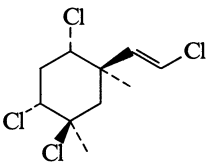
Constit. of *Schisandra sphenanthera*. Cryst. (Et_2O/hexane). Mp 114-115°.

Yue, J.-M. *et al*, *Phytochemistry*, 1989, **28**, 1774.

Gelidene G-80006

1,2,4-Trichloro-5-(2-chloroethenyl)-1,5-dimethylcyclohexane, 9CI

[123805-38-9]



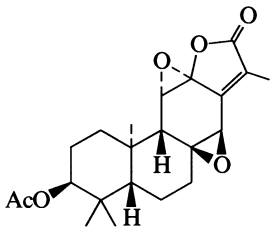
$C_{10}H_{14}Cl_4$ M 276.031

Metab. of *Gelidium sesquipedale*. Cryst. Mp 82°. $[\alpha]_D^{20}$ −55°.

[106621-87-8, 106621-88-9, 106621-89-0, 106621-90-3]

Aazizi, M.A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 829 (*isol, pmr, cmr*)

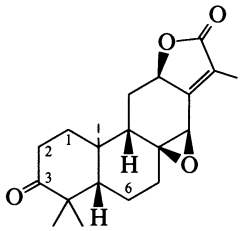
Gelomulide B G-80007



$C_{22}H_{28}O_6$ M 388.460
Constit. of *Gelonium multiflorum*. Needles. Mp 252°. $[\alpha]_D$ +126.7° (c, 0.015 in $CHCl_3$).

Talapatra, S.K. *et al*, *Phytochemistry*, 1989, **28**, 1181.

Gelomulide C G-80008



$C_{20}H_{26}O_4$ M 330.423
Constit. of *Gelonium multiflorum*. Needles. Mp 173°. $[\alpha]_D$ −27° (c, 0.077 in $CHCl_3$).

1β-Acetoxy: ***Gelomulide F***
$C_{22}H_{28}O_6$ M 388.460
Constit. of *G. multiflorum*. Needles. Mp 220°. $[\alpha]_D$ −11° (c, 0.082 in $CHCl_3$).

3-Alcohol, 3-O-Ac: ***Gelomulide A***
$C_{22}H_{30}O_5$ M 374.476
Constit. of *G. multiflorum*. Needles. Mp 240°. $[\alpha]_D$ +95° (c, 0.08 in $CHCl_3$). 3-Config. undetd.

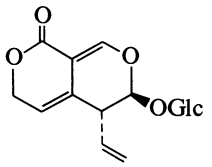
1,2-Didehydro: ***Gelomulide D***
$C_{20}H_{24}O_4$ M 328.407
From *G. multiflorum*. Needles. Mp 220°. $[\alpha]_D$ +7.6° (c, 0.08 in $CHCl_3$).

1,2-Didehydro, 6β-acetoxy: ***Gelomulide E***
$C_{22}H_{26}O_6$ M 386.444
Constit. of *G. multiflorum*. Needles. Mp 241°. $[\alpha]_D$ −12.5° (c, 0.08 in $CHCl_3$).

Talapatra, S.K. *et al*, *Phytochemistry*, 1989, **28**, 1181.

Gentiopicroside G-80009

Updated Entry replacing G-30003
Gentiopicrin
[20831-76-9]



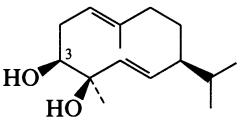
$C_{16}H_{20}O_9$ M 356.329

Widespread in the Gentianaceae, eg. *Swertia* and *Gentiana* spp. Cryst. Mp 191° (from EtOAc), Mp 122° (from H_2O). $[\alpha]_D$ −196.3° (H_2O). The nat. prods. Erytaurin, Gentiamarin and Sabbatin were said to be identical with Gentiopicroside (Korte, 1954-55). However this work is unreliable (Tomita 1960).

Aglucone: Mesogentiogenin
$C_{10}H_{10}O_4$ M 194.187
Oil.

Tomita, Y., *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1960, **81**, 1726 (*pmr, struct*)
Inouye, H. *et al*, *Tetrahedron Lett.*, 1968, 4429 (*pmr, struct*)
Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985 (*occur*)
Das, S. *et al*, *Phytochemistry*, 1984, **23**, 908 (*isol*)

1(10),5-Germacradiene-3,4-diol G-80010

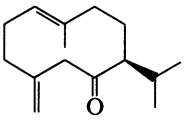


$C_{15}H_{26}O_2$ M 238.369
Leaflets (hexane). Mp 128°. $[\alpha]_D^{25}$ −201° (c, 1.3 in CH_2Cl_2).

3-Ac: 3-Acetoxy-1(10),5-germacradien-4-ol
$C_{17}H_{28}O_3$ M 280.406
Constit. of *Pallenis spinosa*. Needles (hexane). Mp 113°. $[\alpha]_D^{25}$ −145° (c, 0.8 in CH_2Cl_2).

Appendino, G. *et al*, *Phytochemistry*, 1989, **28**, 849.

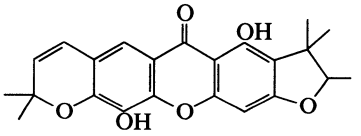
1(10),4(15)-Germacradien-6-one G-80011



$C_{15}H_{24}O$ M 220.354
Constit. of *Baccharis latifolia*. Oil.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

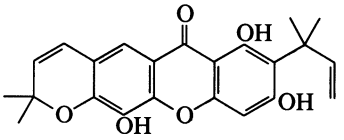
Gerontoxanthone A G-80012



$C_{23}H_{22}O_6$ M 394.423
Constit. of *Cudrania cochinchinensis*. Yellow needles (EtOAc). Mp 236-238°. $[\alpha]_D$ −22.12° (c, 0.6 in $CHCl_3$).

Chang, C.-H. *et al*, *Phytochemistry*, 1989, **28**, 595.

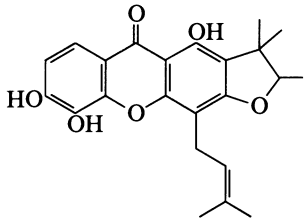
Gerontoxanthone B G-80013



$C_{23}H_{22}O_6$ M 394.423
Constit. of *Cudrania cochinchinensis*. Yellow needles (EtOAc). Mp 216-218°.

Chang, C.-H. *et al*, *Phytochemistry*, 1989, **28**, 595.

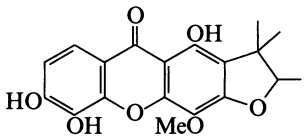
Gerontoxanthone C G-80014



$C_{23}H_{24}O_6$ M 396.439
Constit. of *Cudrania cochinchinensis*. Pale yellow needles (MeOH). Mp 204-206°.

Chang, C.-H. *et al*, *Phytochemistry*, 1989, **28**, 595.

Gerontoxanthone D G-80015

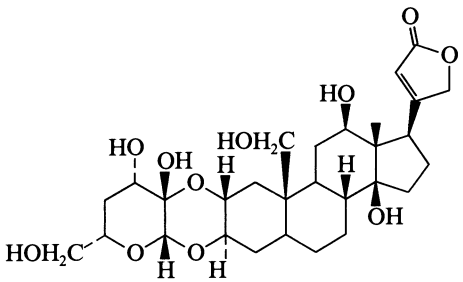


$C_{19}H_{18}O_7$ M 358.347
Constit. of *Cudrania cochinchinensis*. Yellow needles (MeOH). Mp 300°.

Chang, C.-H. *et al*, *Phytochemistry*, 1989, **28**, 595.

Ghalakinoside G-80016

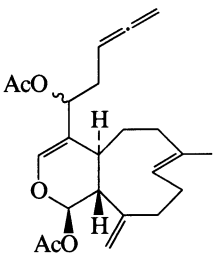
[119459-76-6]



$C_{29}H_{42}O_{11}$ M 566.644
Constit. of *Pergularia tomentosa*. A cytotoxic cardiac glycoside. Cryst. (MeOH). Mp 215-220°. $[\alpha]_D^{25}$ +60°.

Al-Said, M.-S. *et al*, *Phytochemistry*, 1988, **27**, 3245 (*isol, cryst struct*)

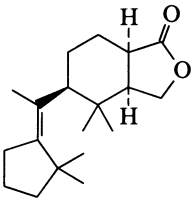
Ginamallene G-80017



$C_{23}H_{30}O_5$ M 386.487
Constit. of *Acalycigorgia* spp. Oil. $[\alpha]_D$ +53° (c, 1.05 in $CHCl_3$).

Fusetani, N. *et al*, *Tetrahedron*, 1989, **45**, 1647.

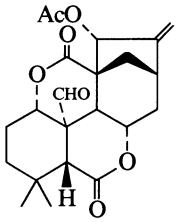
Glaciolide G-80018



$C_{19}H_{30}O_2$ M 290.445
Constit. of nudibranch *Cadlina luteomarginata* and the sponge *Aplysilla glacialis*. Needles (hexane). Mp 102-103°. $[\alpha]_D$ +18.9° (c, 0.14 in EtOH).

Tischler, M. *et al*, *Tetrahedron Lett.*, 1989, **30**, 5717.

Glaucocalactone G-80019



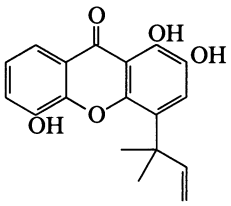
$C_{22}H_{26}O_7$ M 402.443
Constit. of *Rabdosia japonica*. Prisms (CH_2Cl_2). Mp 318-320° dec.

Meng, X. *et al*, *Phytochemistry*, 1989, **28**, 1163 (*isol, cryst struct*)

Globuxanthone G-80020

4-(1,1-Dimethyl-2-propenyl)-1,2,5-trihydroxy-9H-xanthen-9-one, 9CI

[13586-28-2]



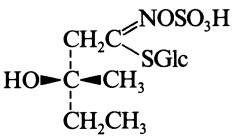
$C_{18}H_{16}O_5$ M 312.321
Isol. from heartwood of *Symphonia globulifera*. Orange needles (C_6H_6). Mp 162-163°.

Tri-Me ether: [13797-87-0]. Mp 125.5°.

Locksley, H.D. *et al*, *J. Chem. Soc. C*, 1966, 430, 2186 (*isol, uv, ir, pmr, ms*)

Glucocleomin G-80021

[36286-64-3]



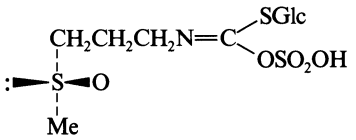
$C_{12}H_{23}NO_{10}S_2$ M 405.446
Isol. from seeds of *Cleome spinosa* and from *Capparis* sp.

Kjaer, A. *et al*, *Acta Chem. Scand.*, 1962, **16**, 591; 1963, **17**, 279 (*isol, struct, abs config*)
Ahmed, Z.F. *et al*, *Phytochemistry*, 1972, **11**, 251 (*isol*)

Glucoiberin G-80022

1-Thio-β-D-glucopyranoside 1-[4-(methylsulfinyl)]N-(sulfooxy)butanimidate, 9CI

[554-88-1]



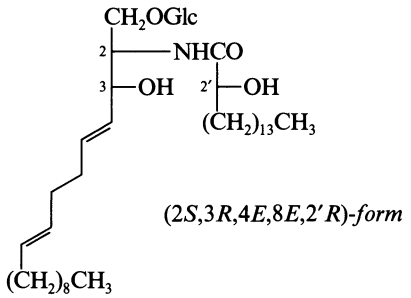
$C_{11}H_{21}NO_{10}S_3$ M 423.486

Isol. from seeds of *Iberis amata*, *Brassica oleracea* and other crucifers. Needles (EtOH aq.). Mp 142-144°. $[\alpha]_D^{20}$ −55.3° (H_2O).

Schutz, O.E. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1954, 404 (*isol, struct*)

Benkert, K., *Naturwissenschaften*, 1966, **53**, 200 (*isol*)

1-*O*-β-D-Glucopyranosyl-*N*-(2-hydroxyhexadecanoyl)-4,8-sphingadiene G-80023



$C_{40}H_{75}NO_9$ M 714.034

(2S,3R,4E,8E,2′R)-form [114297-20-0]

Cerebroside isol. from *Tetragonia tetragonoides* (Tetragoniae Herba). Antiulcerogenic principle. Hygroscopic granules. Mp 184-186°. $[\alpha]_D^{24}$ +10.5° (c, 0.30 in MeOH/$CHCl_3$, 3:2).

(2S,3R,4E,8Z,2′R)-form [115074-93-6]

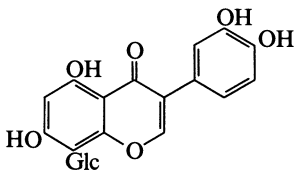
Isol. from *T. tetragonoides*. Antiulcerogenic principle. Hygroscopic granules. Mp 192-194° (183°). $[\alpha]_D^{24}$ +13.4° (c, 0.43 in MeOH/$CHCl_3$ 3:2)(+4.6°).

Mori, K. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 807 (*abs config, ir, pmr, cmr, synth, bibl*)

8-*C*-Glucosyl-3′,4′,5,7-tetrahydroxyisoflavone G-80024

Orobol 8-C-glucoside. 8-C-β-D-Glucopyranosylorobol

[66026-81-1]



$C_{21}H_{20}O_{11}$ M 448.382

Isol. from bark of *Dalbergia nitidula* and flowers of *Lupinus luteus*. Light-yellow amorph. solid. Mp 190-193°, Mp 265°. $[\alpha]_D$ + ±0° (MeOH/Py 1:1).

Octa-Ac: Amorph. solid. Mp 120°, Mp 132-134°.

3′-Me ether: [40522-83-6]. *8-C-Glucosyl-4′,5,7-trihydroxy-3′-methoxyisoflavone.* ***Dalpanitin***

$C_{22}H_{22}O_{11}$ M 462.409

Isol. from seeds of *D. paniculata*. Rectangular plates + $1\frac{1}{2}H_2O$. Mp 213-214° dec. $[\alpha]_D$ +35° (c, 0.73 in EtOH).

Adinarayana, D. *et al*, *Tetrahedron*, 1972, **28**, 5377 (*Dalpanitin*)

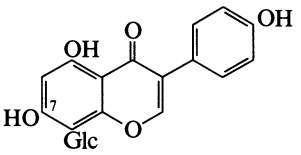
Zapesochnaya, G.G. *et al*, *Khim. Prir. Soedin.*, 1977, **13**, 862; *cnc*, 729 (*isol, pmr, struct*)

Van Heerden, F.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 2463 (*isol, cmr*)

8-*C*-Glucosyl-4′,5,7-trihydroxyisoflavone G-80025

Genistein 8-C-glucoside. 8-C-Glucopyranosylgenistein

[66026-80-0]



$C_{21}H_{20}O_{10}$ M 432.383

Isol. from bark of *Dalbergia nitidula* and from most organs of *Lupinus luteus*. Light-yellow amorph. solid. Monohydrate (MeOH aq.). Mp 185-189°, Mp >350°. $[\alpha]_D^{20}$ +24° (c, 1 in MeOH). Wide discrepancy in Mp's, no comparison of samples.

Hepta-O-Ac: Light-yellow amorph. solid. Mp 108-110°.

7-Me ether: [52448-12-1]. *8-C-Glucosyl-4′,5-dihydroxy-7-methoxyisoflavone. Prunetin 8-C-glucoside. 8-C-Glucosylprunetin*

$C_{22}H_{22}O_{10}$ M 446.410

Isol. from bark of *D. paniculata*. Plates + $1H_2O$ (MeOH). Mp 286-287°.

Parthasarathy, M.R. *et al*, *Phytochemistry*, 1976, **15**, 1025 (*isol, uv, ir, ms, deriv*)

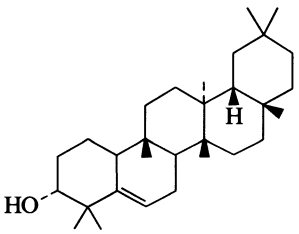
Zapesochnaya, G.G. *et al*, *Khim. Prir. Soedin.*, 1977, 862; *Chem. Nat. Compd.* (*Engl. Transl.*), 729 (*isol, pmr*)

Van Heerden, F.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 2463 (*isol, cmr*)

5-Gluten-3-ol G-80026

Updated Entry replacing G-70020

D:B-Friedoolean-5-en-3-ol, 9CI



$C_{30}H_{50}O$ M 426.724

3α-form [14554-13-3] ***Alnusenol.*** *Glutinol*

Constit. of *Euphorbia cyparissias* and *E. royleana*. Cryst. (MeOH). Mp 210.5-211.5° (203-205°). $[\alpha]_D$ +61° (c, 1 in $CHCl_3$).

3β-form [545-24-4]

Constit. of *E.* spp. Cryst. (MeOH/$CHCl_3$). Mp 210-213°. $[\alpha]_D^{23}$ +63.3° (c, 0.71 in $CHCl_3$).

Ac:

$C_{32}H_{52}O_2$ M 468.762

Constit. of *E. maculata*. Needles (MeOH/$CHCl_3$). Mp 190-191.5°. $[\alpha]_D^{23}$ +76.8° (c, 0.5 in $CHCl_3$).

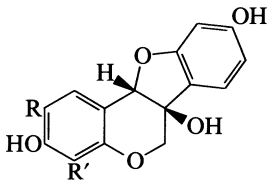
Sengupta, P. *et al*, *J. Indian Chem. Soc.*, 1965, **42**, 543 (*isol*)

Starratt, A.N., *Phytochemistry*, 1966, **5**, 1341 (*isol*)

Matsunaga, S. *et al*, *Phytochemistry*, 1988, **27**, 535 (*isol*)

Glyceollidin I G-80027

3,6a,9-Trihydroxy-4-(3-methyl-2-butenyl)pterocarpan. 4-(Dimethylallyl)trihydroxypterocarpan. 4-Isopentenyl-3,6a,9-trihydroxypterocarpan



R = H, R′ = – $CH_2CH{=}C(CH_3)_2$

Absolute configuration

$C_{20}H_{20}O_5$ M 340.375

No opt. rotn. reported. Phytoalexin from *Glycine max*.

Zähringer, U. *et al*, *Z. Naturforsch.*, *C*, 1981, **36**, 234.

Glyceollidin II G-80028

*2-(3-Methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,6*a*,9(11*a*H)triol, 9CI. 2-Isopentenyl-3,6*a*,9-trihydroxypterocarpan. 2-(Dimethylallyl)trihydroxypterocarpan. Glyceocarpin*

[77979-22-7]

As Glyceollidin I, G-80027 with

R = $-CH_2CH{=}C(CH_3)_2$, R′ = H

$C_{20}H_{20}O_5$ M 340.375

Phytoalexin from *Glycine max*.

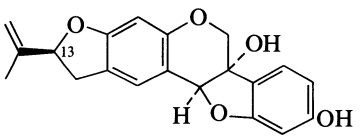
Ingham, J.L. *et al*, *Phytochemistry*, 1981, **20**, 795 (*isol*, *struct*, *abs config*)

Zähringer, U. *et al*, *Z. Naturforsch.*, *C*, 1981, **36**, 234 (*isol*)

Glyceollin III G-80029

Updated Entry replacing G-30013

[67314-02-7]



$C_{20}H_{18}O_5$ M 338.359

Phytoalexin from *Glycine max*. Also from *G. gracilis*, *G. latrobeana* and *G. soja*. Cryst. (EtOH aq.). Mp 149-153°.

13-Epimer: [79082-46-5]. ***Canescacarpin***

$C_{20}H_{18}O_5$ M 338.359

Isol. from leaves of *Glycine canescens*. Cryst. (EtOH). Mp 164-167°.

Lyne, R.L. *et al*, *J. Chem. Soc.*, *Chem. Commun.*, 1976, 497 (*isol*)

Lyne, R.L. *et al*, *Tetrahedron Lett.*, 1981, 2483 (*Canescacarpin*)

Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*occur*)

Banks, S.W. *et al*, *Phytochemistry*, 1983, **22**, 2729 (*biosynth*)

Glycolloglycollic acid G-80030

Carboxymethyl hydroxyacetate, 9CI. Glycolic acid bimol. ester, 8CI

[30450-85-2]

$HOCH_2COOCH_2COOH$

$C_4H_6O_5$ M 134.088

Prisms (EtOAc). Sol. H_2O, AcOH. Mp 99-100°.

Wolf, L. *et al*, *Justus Liebigs Ann. Chem.*, 1900, **312**, 146 (*synth*)

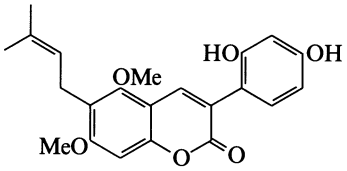
Fischer, H.O.L. *et al*, *Helv. Chim. Acta*, 1933, **16**, 1130 (*synth*)

Micheau, J.C. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 4018 (*synth*, *pmr*, *ir*)

Glycyrin G-80031

*3-(2,4-Dihydroxyphenyl)-5,7-dimethoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, 9CI. 3-(2,4-Dihydroxyphenyl)-5,7-dimethoxy-6-prenylcoumarin*

[66056-18-6]



$C_{22}H_{22}O_6$ M 382.412

Isol. from roots of *Glycyrrhiza* sp. (licorice). Yellow needles. Mp 209-211°.

Kinoshita, T. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 135 (*isol*, *uv*, *pmr*, *struct*)

Gold's reagent G-80032

N-[[[(Dimethylamino)methylene]amino]methylene]-N-methylmethanaminium(1+), 9CI. [[[(Dimethylamino)methylene]amino]methylene]dimethylammonium(1+), 8CI

$Me_2N^{\oplus}{=}CHN{=}CHNMe_2$

$C_6H_{14}N_3^{\oplus}$ M 128.197

Intermed. for triazoles, triazines.

Chloride: [20353-93-9].

$C_6H_{14}ClN_3$ M 163.649

Tan solid (Me_2CO). Mp 103°.

Hexachloroantimonate: [104543-47-7].

$C_6H_{14}Cl_6N_3Sb$ M 462.663

Yellow prisms (MeOH). Mp 133-135°.

Perchlorate: [87112-29-6].

$C_6H_{14}ClN_3O_4$ M 227.647

Cryst. (EtOH). Mp 110-111°.

[50781-48-1]

Krchnak, V. *et al*, *Collect. Czech. Chem. Commun.*, 1974, **39**, 3327; 1975, **40**, 1384 (*synth*, *ir*, *uv*)

Kantlehner, W. *et al*, *Justus Liebigs Ann. Chem.*, 1979, 528 (*synth*, *pmr*)

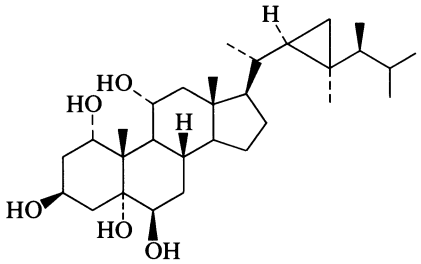
Gupton, J.T., *J. Org. Chem.*, 1980, **45**, 4522 (*synth*, *pmr*)

Gould, R.O. *et al*, *Acta Crystallogr.*, *Sect. C*, 1983, **39**, 1097 (*cryst struct*)

Mueller, E. *et al*, *Tetrahedron*, 1985, **41**, 5901 (*synth*, *ir*, *pmr*, *uv*)

Gupton, J.T., *Aldrichimica Acta*, 1986, **19**, 43 (*rev*)

1,3,5,6,11-Gorgostanepentol G-80033



$C_{30}H_{52}O_5$ M 492.738

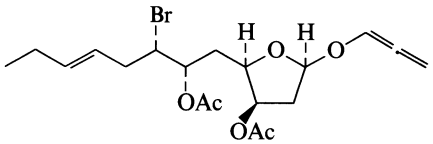
(1α,3β,5α,6β,11α)-form [117569-43-4]

Constit. of *Iris hippuris*. Cryst. Mp 295-297°.

Rao, C.B. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 954.

Graciosallene G-80034

[119285-22-2]



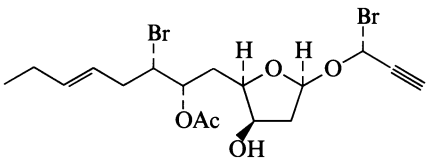
$C_{19}H_{27}BrO_6$ M 431.323

Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ −83.3° (c, 0.018 in $CHCl_3$).

Norté, M. *et al*, *Phytochemistry*, 1988, **27**, 3537.

Graciosin G-80035

[119285-19-7]



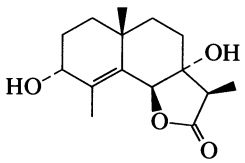
$C_{17}H_{24}Br_2O_5$ M 468.182

Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ −14.5° (c, 0.62 in $CHCl_3$).

González, A.G. *et al*, *Tetrahedron*, 1984, **40**, 3443 (*isol*)

Norte, M. *et al*, *Phytochemistry*, 1988, **27**, 3537 (*isol, cryst struct*)

Grangolide G-80036



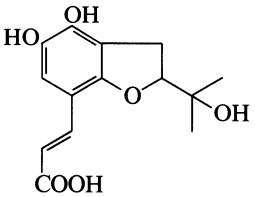
$C_{15}H_{22}O_4$ M 266.336

Constit. of *Grangea maderspatana*. Cryst. Mp 135-139°. $[\alpha]_D^{24}$ +12° (c, 2.76 in $CHCl_3$).

Ruangrungsi, N. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 130.

Gravolenic acid G-80037

[13781-46-9]



$C_{14}H_{16}O_6$ M 280.277

Isol. from above-ground parts of *Ruta graveolens*. Light-yellow cryst. (EtOAc or Me_2CO aq.). Mp 194°.

Reisch, J. *et al*, *Acta Pharm. Suec.*, 1966, **3**, 423 (*pmr, ord*)

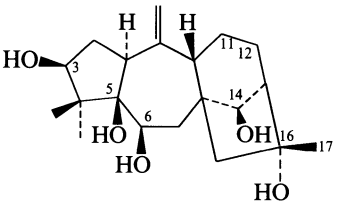
Novák, I. *et al*, *Planta Med.*, 1966, **14**, 151 (*isol, uv, ir, struct*)

Grayanotoxin II G-80038

Updated Entry replacing G-00665

*10(20)-Grayanotoxene-3β,5β,6β,14*R*,16α-pentol*

[4678-44-8]



$C_{20}H_{32}O_5$ M 352.470

Toxic substance from the leaves of *Leucothoe grayana*. Cryst. (EtOAc). Mp 197-198°. $[\alpha]_D^{28}$ −41.9°. Substances known as Asebotoxin, Rhodotoxin and Andromedotoxin as well as Grayanotoxin were isolated from various plants before 1960 and mostly consisted of Grayanotoxins or mixtures.

▷ PB9220000.

6-Ac: [59236-87-2]. ***Grayanotoxin XVI***

$C_{22}H_{34}O_6$ M 394.507

Constit. of *L. grayana*. Cryst. (Et_2O). Mp 116-118°. $[\alpha]_D$ +28° (c, 1 in MeOH).

14-Ac: [30272-17-4]. ***Grayanotoxin IV***

$C_{22}H_{34}O_6$ M 394.507

Constit. of *L. grayana*. Cryst. (EtOAc). Mp 174-175°. $[\alpha]_D$ −18.6° (c, 1 in MeOH).

▷ PB9221000.

O⁶-Ac, O³-β-D-Glucopyranoside: [69842-18-8]. ***Grayanoside A***

$C_{28}H_{44}O_{11}$ M 556.649

Constit. of *L. grayana*. Syrup. $[\alpha]_D^{25}$ −19.1° (c, 2.35 in MeOH).

11α-Hydroxy: [35928-08-6]. ***Grayanotoxin XII.*** *10(20)-Grayanotoxene-3β,5β,6β,11α,14*R*,16α-hexol*

$C_{20}H_{32}O_6$ M 368.469

Constit. of *L. grayana*. Cryst. Mp 208-209°.

12β-Hydroxy: [33880-98-7]. ***Grayanotoxin XI.*** *10(20)-Grayanotoxene-3β,5β,6β,12β,14*R*,16α-hexol*

$C_{20}H_{32}O_6$ M 368.469

Constit. of *L. grayana*. Cryst. Mp 176-177°.

12β-Hydroxy,14-Ac: [35928-07-5]. ***Grayanotoxin XIII***

$C_{22}H_{34}O_7$ M 410.506

Constit. of *L. grayana*. Cryst. Mp 150-151°.

Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985, no. 3678 (*bibl*)

Kakisawa, H. *et al*, *Tetrahedron Lett.*, 1962, 215 (*struct*)

Yasue, M. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 2586 (*stereochem*)

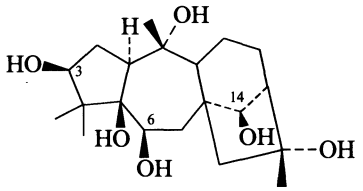
Okuno, T. *et al*, *Tetrahedron*, 1970, **26**, 4765 (*struct*)
Hikino, H. *et al*, *Chem. Pharm. Bull.*, 1971, **19**, 1289; 1972, **20**, 422 (*Grayanotoxin XI, Grayanotoxin XII, Grayanotoxin XIII*)
Gasa, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 835 (*isol*)
Gasa, S. *et al*, *Tetrahedron Lett.*, 1976, 553 (*synth*)
Sakakibara, J. *et al*, *Phytochemistry*, 1978, **17**, 1672 (*Grayanoside A*)
Furusaki, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 1956 (*cryst struct*)

Grayanotoxin III G-80039

Updated Entry replacing G-00666

*3β,5β,6β,10α,14*R*,16α-Grayanotoxanehexol. Andromedol*

[4678-45-9]



$C_{20}H_{34}O_6$ M 370.485

Toxic constit. of *Leucothoe grayana*. Cryst. + ½ EtOAc. Mp 218° dec. $[\alpha]_D^{15}$ −12°.

▷ Toxic. PB9190000.

14-Ac: [4720-09-6]. ***Grayanotoxin I.*** *Acetylandromedol*
$C_{22}H_{36}O_7$ M 412.522
Toxic agent from *Rhododendron*, *Kalmin*, *Leucothoe* and *Lyonia* spp. Cryst. (EtOAc/pentane). Mp 267-270°. $[\alpha]_D^{25}$ −8.8° (c, 2.3 in EtOH).
▷ PB9195000.

6,14-Di-Ac: [30460-34-5]. ***Rhodojaponin IV***
$C_{24}H_{38}O_8$ M 454.559
Constit. of *Rhododendron* spp. Cryst. Mp 245-247°.

3-Ketone: [30272-18-5]. ***Grayanotoxin V.*** *5β,6β,10α,14*R*,16α-Pentahydroxygrayanotoxan-3-one*
$C_{20}H_{32}O_6$ M 368.469
Constit. of *L. grayana* leaves. Cryst. (EtOAc). Mp 230-232° dec. $[\alpha]_D$ −61.5° (c, 1 in MeOH).

3-Ketone,14-Ac: [39012-12-9]. ***Grayanotoxin XIV***
$C_{32}H_{34}O_7$ M 530.616
Constit. of *L. grayana*. Cryst. Mp 242-243°. $[\alpha]_D$ −51° (c, 1 in MeOH).

3,6-Diketone: [59740-27-1]. ***Grayanotoxin XVII.*** *5β,10α,14*R*,16α-Tetrahydroxy-3,6-grayanotoxanedione*
$C_{20}H_{30}O_6$ M 366.453
Constit. of *L. grayana*. Cryst. (MeOH). Mp 268-270° dec. $[\alpha]_D$ −157.3° (c, 1 in MeOH).

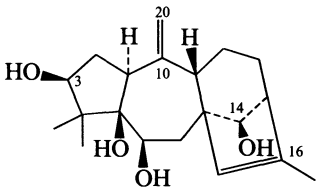
Tallent, W.H. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 4548 (*struct*)
Kakisawa, H. *et al*, *Tetrahedron Lett.*, 1962, 215 (*struct*)
Hikino, H. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 1071, 2357 (*stereochem, isol*)
Okuno, T. *et al*, *Tetrahedron*, 1970, **26**, 4765 (*isol*)
Narayanan, P. *et al*, *Tetrahedron Lett.*, 1970, 3943 (*cryst struct*)
Hamanaka, N. *et al*, *Chem. Lett.*, 1972, 779 (*isol*)
Gasa, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 835 (*Grayanotoxin XVII*)
Jawad, F.H. *et al*, *Biomed. Mass Spectrom.*, 1977, **4**, 331 (*ms*)
Masutani, T. *et al*, *Agric. Biol. Chem.*, 1979, **43**, 631 (*cmr*)

Grayanotoxin VII G-80040

Updated Entry replacing G-00669

*10(20),15-Grayanotoxadiene-3β,5β,6β,14*R*-tetrol*

[30460-59-4]



$C_{20}H_{30}O_4$ M 334.455

Constit. of *Leucothoe grayana*. Cryst. Mp 187-189°.

▷ PB9240000.

14-Ac: [30460-58-3]. ***Grayanotoxin IX***
$C_{22}H_{32}O_5$ M 376.492
Constit. of *L. grayana*. Cryst. Mp 151-152°.

Δ^{16}*-Isomer:* [30460-60-7]. ***Grayanotoxin VIII.*** *10(20),16-Grayanotoxadiene-3β,5β,6β,*14R*-tetrol*
$C_{20}H_{30}O_4$ M 334.455
Constit. of *L. grayana*. Cryst. Mp 190-193°.

Δ^{16}*-Isomer,14-Ac:* [36660-75-0]. ***Grayanotoxin X***
$C_{22}H_{32}O_5$ M 376.492
Constit. *L. grayana*. Mp 165.5-166.5°.

10,20-Dihydro,10α-hydroxy: [30460-36-7]. ***Grayanotoxin VI.*** *15-Grayanotoxene-3β,5β,6β,*10α,14R*-pentol*
$C_{20}H_{32}O_5$ M 352.470
Constit. of *L. grayana*. Cryst. Mp 219-221°.

14-Deoxy: [75829-08-2]. ***Grayanotoxin XIX.*** *10(20),15-Grayanotoxadiene-3β,5β,6β-triol*
$C_{20}H_{30}O_3$ M 318.455
Constit. of *L. grayana*. Cryst. (Et_2O). Mp 132-133°. $[\alpha]_D$ −12° (c, 1 in MeOH).

3-Ketone: [78534-58-4]. ***Grayanotoxin XX.*** *5β,6β,*14R*-Trihydroxy-*10(20),15*-grayanotoxadien-*3*-one*
$C_{20}H_{28}O_4$ M 332.439
Data inaccessible.

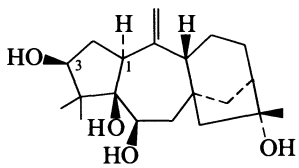
Hikino, H. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 2357; 1971, **19**, 1289 (*isol*)
Furusaki, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 1622 (*cryst struct, Grayanotoxin XIX*)

Grayanotoxin XVIII G-80041

Updated Entry replacing G-00675

10(20)Grayanotoxene-3β,5,6β,16-tetrol

[70474-76-9]



$C_{20}H_{32}O_4$ M 336.470

Constit. of *Leucothoe grayana*. Cryst. (diisopropyl ether). Mp 162-164°. $[\alpha]_D^{25}$ −6.8° (c, 2.2 in MeOH).

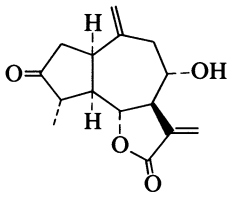
3-O-β-D-Glucopyranoside: [70474-75-8]. ***Grayanoside* B**
$C_{26}H_{42}O_9$ M 498.612
Constit. of *L. grayana*. Viscous syrup. $[\alpha]_D^{16}$ −14.1° (c, 2.6 in MeOH).

1-Epimer, 3-O-β-D-glucopyranoside: [74311-31-2]. ***Grayanoside C***
$C_{26}H_{42}O_9$ M 498.612
Isol. from *L. grayana*. Syrup. Mp 220-222° (as pentaacetate). $[\alpha]_D^{24}$ +6.0° (c, 2 in MeOH).

Sakakibara, J. *et al*, *Phytochemistry*, 1979, **18**, 135; 1980, **19**, 1495 (*isol, struct, pmr*)
Furusaki, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 657 (*cryst struct*)

Grosheimin G-80042

Updated Entry replacing G-00696
[22489-66-3]

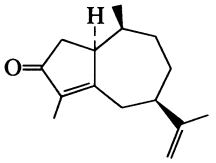


$C_{15}H_{18}O_4$ M 262.305
Constit. of *Chartolepsis intermedia* and *Grossheimia macrocephala*. Cryst. (MeOH). Mp 205°. $[\alpha]_D^{20}$ +137.7° (c, 0.2 in MeOH).

3α-Alcohol: ***Grosheiminol***
$C_{15}H_{20}O_4$ M 264.321
Constit. of *G. macrocephala*. Oil. $[\alpha]_D^{25}$ +56.4° (c, 0.1 in Py).

Samek, Z. *et al*, *Collect. Czech. Chem. Commun.*, 1972, **37**, 2611.
Daniewski, W. *et al*, *Collect. Czech. Chem. Commun.*, 1982, **47**, 3160 (*Grosheiminol*)

4,11(13)-Guaiadien-3-one G-80043

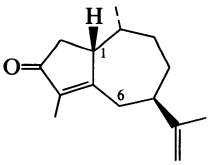


$C_{15}H_{22}O$ M 218.338
Constit. of *Baccharis boliviensis*. Oil. $[\alpha]_D^{24}$ +63° (c, 0.23 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

4,11-Guaiadien-3-one G-80044

[7764-53-6]

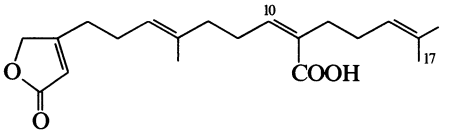


$C_{15}H_{22}O$ M 218.338
Constit. of *Pleocarphus revolutus*. Oil. $[\alpha]_D^{24}$ −63° (c, 0.75 in $CHCl_3$).

1β-Hydroxy, 6β-acetoxy: [116085-10-0]. *6β-Acetoxy-1β-hydroxy-4,11-guaiadien-3-one*
$C_{17}H_{24}O_4$ M 292.374
Constit. of *P. revolutus*.

Büchi, G. *et al*, *Proc. Chem. Soc., London*, 1962, 280 (*synth*)
Zdero, C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 509.

Gutiesolbriolide G-80045



$C_{20}H_{28}O_4$ M 332.439
Parent compd. unknown.

17-Hydroxy: ***17-Hydroxygutiesolbriolide***
$C_{20}H_{28}O_5$ M 348.438
Constit. of *Gutierrezia solbrigii*.

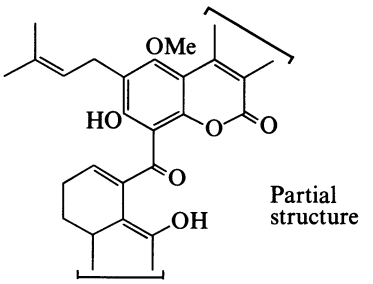
17-Hydroxy, 10E-isomer:
$C_{20}H_{28}O_5$ M 348.438
Condit. of *G. solbrigii*.

17-Acetoxy: ***17-Acetoxygutiesolbriolide***
$C_{22}H_{30}O_6$ M 390.475
Constit. of *G. solbrigii*.

Jakupovic, J. *et al*, *Tetrahedron*, 1985, **41**, 4537.

α-Guttiferin G-80046

Updated Entry replacing G-60040
[11048-92-3]



$C_{33}H_{38}O_8$ M 562.658
In *CA*, α-Guttiferin is confused with α_2- Guttiferin which is identical with Morellic acid. Constit. of Gamboge the resinous exudation of *Garcinia morella*. Mp 113-115°. $[\alpha]_D^{26}$ −475° (c, 1.5 in $CHCl_3$).

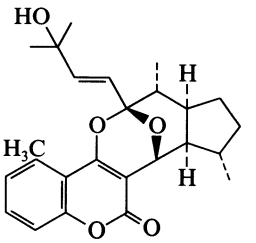
▷ MG1578700.

Py complex: Mp 115-117°. $[\alpha]_D^{26}$ −561.2° (c, 1.496 in $CHCl_3$).

Nageswara Rao, K.V. *et al*, *Experientia*, 1961, **17**, 213 (*struct*)

Gypothamniol G-80047

Updated Entry replacing G-70037



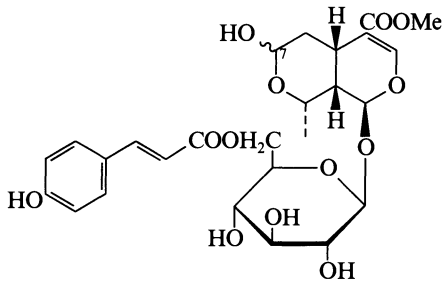
$C_{25}H_{30}O_5$ M 410.509
Constit. of *Gypothamnium pinifolium*. Oil. $[\alpha]_D^{24}$ +58° (c, 0.44 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1988, **27**, 2953.

H

Haenkeanoside H-80001

[119944-56-8]



$C_{26}H_{32}O_{13}$ M 552.531
Constit. of *Isertia haenkeana*.

7-Me ether: [119944-57-9]. **O-*Methylhaenkeanoside***
$C_{27}H_{34}O_{13}$ M 566.558
Constit. of *I. haenkeana*.

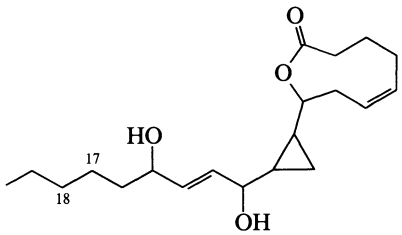
Z-isomer: [119943-44-1]. ***Isohaenkeanoside***
$C_{26}H_{32}O_{13}$ M 552.531
Constit. of *I. haenkeana*.

Z-isomer, 7-Me ether: [119864-05-0]. **O-*Methylisohaenkeanoside***
$C_{27}H_{34}O_{13}$ M 566.558
Constit. of *I. haenkeana*.

[119864-04-9, 119943-43-0, 119943-47-4, 119944-58-0]

Rumbero-Sánchez, A. *et al*, *Heterocycles*, 1988, **27**, 2863.

Halicholactone H-80002



$C_{20}H_{32}O_4$ M 336.470
Metab. of sponge *Halichondria okadai*. Oil. $[\alpha]_D^{23}$ −85.4° (c, 1.16 in $CHCl_3$).

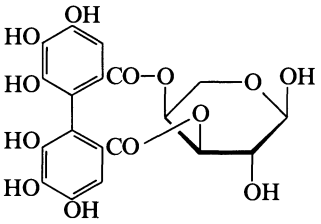
17Z,18-Didehydro: ***Neohalicholactone***
$C_{20}H_{30}O_4$ M 334.455
Metab. of *H. okadai*. Cryst. (Et_2O/pentane). Mp 69-70°. $[\alpha]_D^{16}$ −54.2° (c, 0.73 in $CHCl_3$).

Niwa, H. *et al*, *Tetrahedron Lett.*, 1989, **30**, 4543.

Heaxahydroxydiphenic acid α-L-arabinosediyl ester H-80003

Arabinopyranose cyclic 3,4-(4,4',5,5',6,6'-hexahydroxydiphenate), 8CI

[19833-16-0]

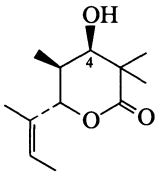


$C_{19}H_{16}O_{13}$ M 452.328
Isol. from fruits of *Psidium guava*. Plates (EtOH aq.). Mp 230-235° dec. $[\alpha]_D^{25}$ −24.2° (c, 0.4 in Py).

Misra, K. *et al*, *Phytochemistry*, 1968, **7**, 641.

Helicascolide A H-80004

[121350-98-9]



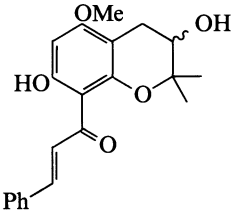
$C_{12}H_{20}O_3$ M 212.288
Metab. of *Helicascus kanaloanus*. Cryst. Mp 97-98°. $[\alpha]_D^{31}$ −25.0° (c, 1.4 in $CHCl_3$).

4-Epimer: [121325-38-0]. ***Helicascolide B***
$C_{12}H_{20}O_3$ M 212.288
Metab. of *H. kanoloanus*. Cryst. Mp 61-62°. $[\alpha]_D^{31}$ −27.6° (c, 0.4 in $CHCl_3$).

Poch, G.K. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 257 (*isol, pmr, cmr*)

Helichromanochalcone H-80005

[72247-81-5]

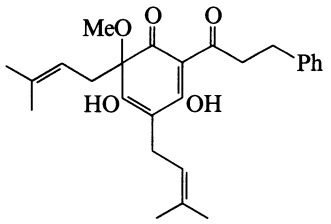


$C_{21}H_{22}O_5$ M 354.402
Isol. from roots of *Helichrysum cymosum*. Yellowish oil.

Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 1033.

Helihumulone H-80006

[72247-83-7]



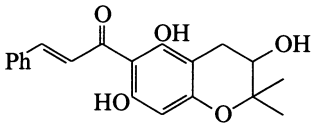
$C_{26}H_{32}O_5$ M 424.536

Isol. from roots of *Helichrysum cymosum*. Oil. $[\alpha]_D^{24}$ +57.8° (c, 1.4 in $CHCl_3$).

Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 1033.

Helikrausichalcone H-80007

[122585-71-1]



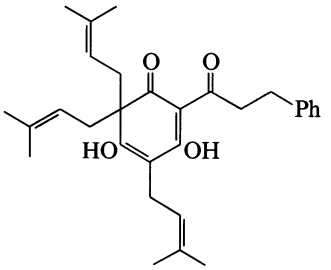
$C_{20}H_{20}O_5$ M 340.375

Constit. of *Helichrysum krausii*. Gum.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

Helilupulone H-80008

[72247-85-9]

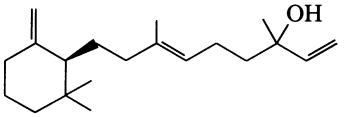


$C_{30}H_{38}O_4$ M 462.628

Isol. from roots of *Helichrysum tenuiculum*. Oil.

Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 1033.

Helipterol H-80009

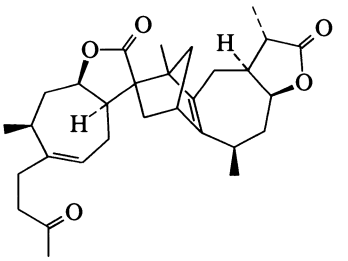


$C_{20}H_{34}O$ M 290.488

Constit. of *Helipterum venustum*. Oil. $[\alpha]_D^{24}$ +13° (c, 0.31 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 517.

Helisplendidilactone H-80010



$C_{30}H_{40}O_5$ M 480.643

Constit. of *Helichrysum splendidum*. Cryst. Mp 172°. $[\alpha]_D^{24}$ −64° (c, 0.21 in $CHCl_3$).

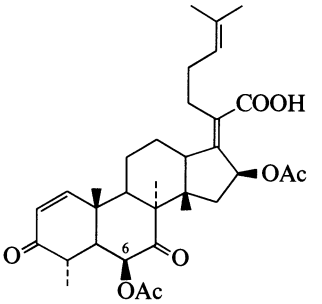
Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

Helvolic acid H-80011

Updated Entry replacing H-00097

6,16-Bis(acetyloxy)-3,7-dioxo-29-nordammara-1,17(20),24-trien-21-oic acid, 9CI. Fumigacin

[29400-42-8]



$C_{33}H_{44}O_8$ M 568.706

Produced by *Aspergillus fumigatus* mut.*helvola*. Shows antibiotic activity against a wide range of organisms, incl. *Staphyloccocus*, *Streptococcus*, *Micrococcus*, *Clostridium*, *Pseudomonas*, *Myobacterium*, *Shigella*, *Salmonella* and*Corynebacterium*. Needles (MeOH). Mp 215°. $[\alpha]_D^{25}$ −121° (c, 1 in $CHCl_3$).

▷ RC1370000.

Me ester: Cryst. (MeOH). Mp 262°. $[\alpha]_D^{23}$ −140° ($CHCl_3$).

Semicarbazone: Mp 240-250° dec.

Dioxime: Needles. Mp 189°.

O^6*-De-Ac:* [10072-61-4]. ***Helvolinic acid***

$C_{31}H_{42}O_7$ M 526.669

Isol. from *Cephalosporium caerulens*, also obt. by mild hydrol. of Helvolic acid. Needles. Mp 202.5-203°. $[\alpha]_D^{24}$ −88.9° (c, 1 in $CHCl_3$).

O^6*-Deacetoxy:* ***6-Deacetoxyhelvolic acid***

$C_{31}H_{42}O_6$ M 510.669

Isol. from culture broth of *C. caerulens*. Needles. Mp 214.5-215°. $[\alpha]_D$ −51.7° (c, 0.5 in $CHCl_3$). Originally descr. as 7-Deacetoxyhelvolic acid prior to the revision of struct. for Helvolic acid.

Allinger, N.L. *et al*, *J. Org. Chem.*, 1961, **26**, 4522 (*uv*, *ir*, *pmr*)
Okuda, S. *et al*, *Chem. Pharm. Bull.*, 1966, **14**, 436 (*6-Deacetoxyhelvolic acid*, *Helvolinic acid*)
Oxley, P., *J. Chem. Soc.*, *Chem. Commun.*, 1966, 729 (*Helvolic acid*)
Okuda, S. *et al*, *Tetrahedron Lett.*, 1967, 2295 (*Helvolic acid*, *struct*)
v. Daehne, W. *et al*, *Tetrahedron Lett.*, 1968, 4843 (*isol*, *nmr*)
Iwasaki, S. *et al*, *J. Chem. Soc.*, *Chem. Commun.*, 1970, 1119 (*struct*, *pmr*)
Cole, R.J. *et al*, *Handbook of Toxic Fungal Metabolites*, Academic Press , N.Y., 1981, 806.

Heneicosanedioic acid H-80012

Updated Entry replacing H-00108

[505-55-5]

$HOOC(CH_2)_{19}COOH$

$C_{21}H_{40}O_4$ M 356.545

Little known. Was descr. (1900) as nat. prod. under the name Japanic acid but this was erroneous.

Lamberton, J.A., *Aust. J. Chem.*, 1961, **14**, 323.

Heneicosanoic acid, 9CI H-80013

[2363-71-5]

$H_3C(CH_2)_{19}COOH$

$C_{21}H_{42}O_2$ M 326.562

Isol. from wood of *Ulex europaeus*, bark of *Pinus contorta*, from *Shorea maranti*, olive oil (*Olea europaea*) etc. Needles (Me_2CO). Mp 73-74°.

[28898-67-1, 59252-40-3]

Le Sueur, H.R. *et al*, *J. Chem. Soc.*, 1915, **107**, 736 (*synth*)
Cocker, W. *et al*, *Perfum. Essent. Oil Rec.*, 1963, **54**, 235 442 (*isol*)
Org. Synth., 1981, **60**, 11 (*synth*)

12,14-Hentriacontanedione, 9CI H-80014

[71149-64-9]

$H_3C(CH_2)_{16}COCH_2CO(CH_2)_{10}CH_3$

$C_{31}H_{60}O_2$ M 464.814

Isol. from wax of *Dianthus caryophyllus* and other plants. Incorr. descr. in one ref. as the 14,16-dione.

Horn, D.H.S. *et al*, *Chem. Ind.* (*London*), 1962, 1036 (*isol*)
Barbieri, G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1987, **50**, 646 (*synth, ir, pmr, cmr, ms*)

14,16-Hentriacontanedione, 9CI H-80015

[24724-84-3]

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_{12}CH_3$

$C_{31}H_{60}O_2$ M 464.814

Isol. from wax of *Eucalyptus risdoni*, *E. coccifera* and other plants.

Horn, D.H.S. *et al*, *Aust. J. Chem.*, 1964, **17**, 464 (*isol*)
Trka, A. *et al*, *Collect. Czech. Chem. Commun.*, 1974, **39**, 468 (*ms*)
Barbieri, G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1987, **50**, 646 (*synth, ir, pmr, cmr, ms*)

Hentriacontanoic acid, 9CI H-80016

[38232-01-8]

$H_3C(CH_2)_{29}COOH$

$C_{31}H_{62}O_2$ M 466.830

Isol. from leaf wax of *Agave sisalana* and other plants. Cryst. (Me_2CO). Mp 93-93.2°.

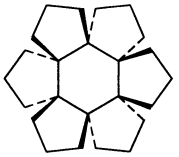
[77630-51-4]

Piper, S.H. *et al*, *Biochem. J.*, 1934, **28**, 2175 (*synth*)
Razafindrazaka, J. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1633 (*isol*)
Rao, S.J. *et al*, *Indian J. Chem., Sect. B*, 1987, **26**, 208 (*synth*)

Heptacyclo[19.3.0.0^{1,5}.0^{5,9}.0^{9,13}.0^{13,17}.0^{17,21}] tetracosane H-80017

[*6.5*]*Coronane*. [*3.3.3.3.3.3*]*Hexannulane*

[106115-42-8]



$C_{24}H_{36}$ M 324.548

Mp 222-224° (subl. from 200°).

Wehle, D. *et al*, *Chem. Ber.*, 1988, **121**, 2171 (*synth, pmr, cmr*)

8,10,12,14-Heptadecatetraen-1-al H-80018

[13894-87-6]

$H_3CCH_2(CH{=}CH)_4(CH_2)_6CHO$

$C_{17}H_{26}O$ M 246.392

Isol. from leaves of *Centaurea* spp. Oil. λ_{max} 279, 291, 304, 319 nm.

(all-E)-form [32507-73-6]

Present in *Zoegea baldshuanica*.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3544; 1971, **104**, 961 (*isol, uv, ir, pmr, struct*)

1,7,9,15-Heptadecatetraene-11,13-diyne, 9CI H-80019

Centaur X_4

[62787-38-6]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH{=}CH(CH_2)_4CH{=}CH_2$

$C_{17}H_{20}$ M 224.345

(E,E,E)-form [34219-14-2]

Isol. from *Dahlia*, *Caiea*, *Gynoxys*, *Heterotheca*, *Bidens*, *Centaurea*, *Senecio*, *Pleiotaxis*, *Coreopsis*, *Calotis* and *Greenmaniella* spp. (all-*E* config. not always specifically indicated). Phytotoxic. Mp 29-30°.

(7E,9E,15Z)-form [22626-80-8]

Isol. from *Aster bellidiastrum*. Oil.

[71608-97-4]

Bohlmann, F. *et al*, *Chem. Ber.*, 1958, **91**, 1624; 1961, **94**, 3179; 1964, **97**, 2135; 1969, **102**, 1034 (*isol, ir, ms, pmr, uv*)
Lam, J. *et al*, *Phytochemistry*, 1971, **10**, 2227 (*occur*)
Bedford, C.T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 735 (*occur*)
Andersen, A.B. *et al*, *Phytochemistry*, 1977, **16**, 1829, 1185 (*isol*)
Bohlmann, F. *et al*, *Phytochemistry*, 1977, **16**, 285, 774, 965, 1065; 1979, **18**, 336, 1185; 1982, **21**, 1434 (*isol*)
Metwally, M.A. *et al*, *Phytochemistry*, 1985, **24**, 182 (*occur*)
Zdero, C. *et al*, *Phytochemistry*, 1987, **26**, 1999; 1988, **27**, 1105 (*occur*)

1,9,15-Heptadecatriene-11,13-diyn-8-ol H-80020

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH(OH)(CH_2)_5CH{=}CH_2$

$C_{17}H_{22}O$ M 242.360

(Z,Z)-form

Isol. from roots of *Cousinia hystrix*. λ_{max} 227, 294, 313 nm (Et_2O).

(9E,15Z)-form [23369-07-5]

Ac: [73631-06-8].

$C_{19}H_{24}O_2$ M 284.397
Found in *Athanasia tridens*. Yellow oil.

Et ether: Yellow oil.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 590; 1967, **100**, 1915 (*isol, struct, synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 1736.

1,9,16-Heptadecatriene-4,6-diyn-3-ol H-80021

[88153-63-3]

$H_2C{=}CH(CH_2)_5CH{=}CHCH_2C{\equiv}CC{\equiv}CCH(OH)CH{=}CH_2$

$C_{17}H_{22}O$ M 242.360

(-)-(*Z*)-*form* [36150-08-0] ***Dehydrofalcarinol***
Isol. from roots of *Artemisia atrata*. Pale-yellow oil. $[\alpha]_D^{23}$ −5.0° (c, 13.9 in Et_2O).

Ac: [78516-98-0].
$C_{19}H_{24}O_2$ M 284.397
Isol. from *Viguiera* sp. Oil.

[13894-97-8]

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3552 (*isol, ir, pmr, struct*)
Bohlmann, F. *et al*, *Phytochemistry*, 1981, **20**, 113 (*isol*)
Harada, R. *et al*, *Phytochemistry*, 1982, **21**, 2009 (*isol*)

2,9,16-Heptadecatriene-4,6-diyn-1-ol H-80022

$H_2C{=}CH(CH_2)_5CH{=}CHCH_2C{\equiv}CC{\equiv}CCH{=}CHCH_2OH$

$C_{17}H_{22}O$ M 242.360

(*Z,Z*)-*form*
Isol. from roots of *Anthemis tinctoria*. Oil. λ_{max} 251.5, 267, 282.5 nm.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2096.

2,9,16-Heptadecatriene-4,6-diyn-8-ol H-80023

$H_2C{=}CH(CH_2)_5CH{=}CHCH(OH)C{\equiv}CC{\equiv}CCH{=}CHCH_3$

$C_{17}H_{22}O$ M 242.360

(*Z,Z*)-*form* [13894-72-9]
Isol. from fresh roots of *Silybum marianum*. Oil. λ_{max} 246.5 (ϵ 4000), 254 (7200), 268.5 (10,400), 284 nm (8000) (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3201 (*isol, uv, ir, pmr, struct*)
Schulz, K.E. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1970, **301**, 7 (*isol*)

1-Heptadecene-4,6-diyne-3,9,10-triol, 9CI H-80024

Panaxytriol

[87005-03-6]

$H_2C{=}CHCH(OH)C{\equiv}CC{\equiv}CCH_2CH(OH)CH(OH)(CH_2)_6CH_3$

$C_{17}H_{26}O_3$ M 278.391
Isol. from *Panax ginseng*. Shows antitumour activity. Needles (H_2O).

Matsunaga, H. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1279 (*isol, uv, pmr, cmr, synth*)

1,5-Heptadiyne, 8CI H-80025

Updated Entry replacing H-00254

[764-56-7]

$HC{\equiv}CCH_2CH_2C{\equiv}CCH_3$

C_7H_8 M 92.140
Bp_{140} 85-90°.

Walba, D.M. *et al*, *J. Org. Chem.*, 1980, **45**, 2259 (*synth, pmr*)

1,1,2,2,3,3,3-Heptafluoro-1-iodopropane, 9CI H-80026

Perfluoro-1-iodopropane

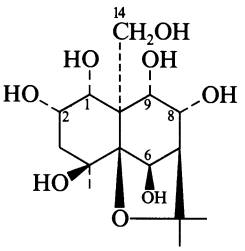
[27636-85-7]

$F_3CCF_2CF_2I$

C_3F_7I M 295.926
Liq. d_4^{20} 2.06. Bp 41.2° (39.5°) . n_D^{20} 1.3272. Turns pink in air.

Hauptschein, M. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 2461 (*synth*)
Haszeldine, R.N., *J. Chem. Soc.*, 1953, 2622 (*uv*)
Nodiff, E.A. *et al*, *J. Org. Chem.*, 1953, **18**, 235 (*props*)
Evans, D.F.E. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 238 (*F nmr*)

1,2,4,6,8,9,14-Heptahydroxydihydro-β-agarofuran H-80027



$C_{15}H_{26}O_8$ M 334.366

(*1α,2α,6β,8α,9α*)-*form*

9-O-*Benzoyl, 1,2,6,8,14-penta-Ac:* ***Celangulin***
$C_{32}H_{40}O_{14}$ M 648.660
Constit. of *Celastrus angulatus*. Insect antifeedant. Amorph. powder.

1,9-Dibenzoyl, 2,6,8,14-tetra-Ac: ***2α,6β,8α,14-Tetraacetoxy-1α,9α-dibenzoyloxy-4β-hydroxydihydro-β-agarofuran***
$C_{37}H_{42}O_{14}$ M 710.730
Constit. of *Maytenus canariensis*. Amorph. solid. Mp 50-52°.

Wakabayashi, N. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 537.
González, A.G. *et al*, *Phytochemistry*, 1989, **28**, 173.

3,3′,4′,5,6,7,8-Heptahydroxyflavone H-80028

Updated Entry replacing H-60024

*2-(3,4-Dihydroxyphenyl)-3,5,6,7,8-pentahydroxy-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{10}O_9$ M 334.239

3′,6,7,8-Tetra-Me ether: 3,4′,5-Trihydroxy-3′,6,7,8-tetramethoxyflavone
$C_{19}H_{18}O_9$ M 390.346
Constit. of *Gymnosperma glutinosum*.

3′,4,5,6,7,8-Hexa-Me ether: [35154-55-3]. *3-Hydroxy-3′,4′,5,6,7,8-hexamethoxyflavone.* ***Natsudaidan***
$C_{21}H_{22}O_9$ M 418.399
Constit. of peel oil of *C. natsudaidai*. Yellow cryst. (EtOH). Mp 154-156° (141-143°).

3′,4,5,6,7,8-Hexa-Me ether, Ac: [35154-56-4].
Mp 125°.

3,3′,4′,6,7,8-Hexa-Me ether: [1176-88-1]. *5-Hydroxy-3,3′,4′,6,7,8-hexamethoxyflavone*
$C_{21}H_{22}O_9$ M 418.399
Isol. from peel of *Citrus sinensis*. Yellow cryst. (MeOH). Mp 110-111°.

3,3′,4,5,8-Penta-Me, 6,7-methylene ether: 3,3′,4,5,8-Pentamethoxy-6,7-methylenedioxyflavone. ***Melicophyllin***
$C_{21}H_{20}O_9$ M 416.384
Constit. of *Melicope triphylla*. Cryst. (Me_2CO). Mp 175-177°.

Sastry, G.P. *et al*, *Tetrahedron*, 1961, **15**, 111 (*synth*)
Row, L.R. *et al*, *Indian J. Chem.*, 1963, **1**, 207 (*synth*)
Gentili, B. *et al*, *Tetrahedron*, 1964, **20**, 2313 (*synth*)
Kinoshita, K. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1971, **91**, 1105 (*isol*)
Tatum, J.H. *et al*, *Phytochemistry*, 1972, **11**, 2283 (*isol, uv*)
Bittner, M. *et al*, *Phytochemistry*, 1983, **22**, 1523 (*isol*)
Yu, S. *et al*, *Phytochemistry*, 1988, **27**, 171 (*isol*)
Jong, T.-T. *et al*, *Phytochemistry*, 1989, **28**, 245 (*isol*)

3′,4′,5,5′,6,7,8-Heptahydroxyflavone H-80029

Updated Entry replacing H-40022

5,6,7,8-Tetrahydroxy-2-(3,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one, 9CI

$C_{15}H_{10}O_9$ M 334.239

4′,5′,6,8-Tetra-Me ether: [18398-74-8]. *3′,5,7-Trihydroxy-4′,5′,6,8-tetramethoxyflavone.* ***Scaposin***
$C_{19}H_{18}O_9$ M 390.346
Isol. from *Hymenoxys scaposa*. Yellow needles ($CHCl_3/C_6H_6$). Mp 210-212°.

4′,5′,6,8-Tetra-Me ether, Tri-Ac: [18398-75-9]. Prisms (MeOH). Mp 179-180°.

4′,6,7,8-Tetra-Me ether: [29550-07-0]. *3′,5,5′-Trihydroxy-4′,6,7,8-tetramethoxyflavone.* ***Gardenin E***
$C_{19}H_{18}O_9$ M 390.346
Isol. from *Gardenia lucida*, *G. turgida* and Dikamali gum. Yellow needles (EtOH). Mp 234°.

4′,6,7,8-Tetra-Me ether, Tri-Ac: [51863-86-6]. Platelets (EtOAc/pet. ether). Mp 163-164°.

3′,4′,5′,6,8-Penta-Me ether: [53950-56-4]. *5,7-Dihydroxy-3′,4′,5′,6,8-pentamethoxyflavone.* ***Luiselizondin***
$C_{20}H_{20}O_9$ M 404.373
Isol. from aerial parts of *Gymnosperma glutinosum*. Yellow needles ($MeOH/CCl_4$). Mp 185-186° (178-179°). Struct. uncertain.

4′,5′,6,7,8-Penta-Me ether: [29550-05-8]. *3′,5-Dihydroxy-4′,5′,6,7,8-pentamethoxyflavone.* ***Gardenin C***
$C_{20}H_{20}O_9$ M 404.373
Isol. from roots of *Gardenia lucida*. Yellow flakes (EtOAc/pet. ether). Mp 179-180°.

3′,4′,5′,6,7,8-Hexa-Me ether: [21187-73-5]. *5-Hydroxy-3′,4′,5′,6,7,8-hexamethoxyflavone.* ***Gardenin A***
$C_{21}H_{22}O_9$ M 418.399
Isol. from roots of *Gardenia turgida* and lead buds of *G. lucida*. Yellow needles (MeOH). Mp 164-165°.

3′,5,5′,6,7,8-Hexa-Me ether: [85644-03-7]. *4′-Hydroxy-3′,5,5′,6,7,8-hexamethoxyflavone*
$C_{21}H_{22}O_9$ M 418.399
Constit. of *Eupatorium leucolepis*. Cryst. ($CHCl_3$/MeOH). Mp 191-193°.

4′,5,5′,6,7,8-Hexa-Me ether: [42557-19-7]. *3′-Hydroxy-4′,5,5′,6,7,8-hexamethoxyflavone*
$C_{21}H_{22}O_9$ M 418.399
Constit. of *E. leucolepis*. Gum.

5,5′,6,8-Tetra-Me, 3′,4′-methylene ether: 7-Hydroxy-5,5′,6,8-tetramethoxy-3′,4′-methylenedioxyflavone
$C_{20}H_{18}O_9$ M 402.357
Constit. of *Ageratum tomentosum* var. *bracteatum*. Yellow cryst. Mp 188-190°.

3,4-Dihydro, hepta-Me ether: 3′,4′,5,5′,6,7,8-Heptamethoxyflavanone
$C_{22}H_{26}O_9$ M 434.442
Constit. of *A. tomentosum* var. *bracteatum*. Yellow gum.

Rao, A.V.R. *et al*, *Indian J. Chem.*, 1968, **6**, 677; 1970, **8**, 398 (*isol, struct, pmr, ms*)
Thomas, M.B. *et al*, *Tetrahedron*, 1968, **24**, 3675 (*isol, synth, uv, ir, pmr, Scaposin*)
Kalra, A.J. *et al*, *Indian J. Chem.*, 1970, **8**, 398; 1973, **11**, 1092 (*isol, synth, uv, pmr*)
Kamalam, M. *et al*, *Indian J. Chem.*, 1970, **8**, 573 (*synth*)
Domínguez, X.A. *et al*, *Phytochemistry*, 1974, **13**, 1624 (*isol, uv, pmr, ms*)
Gupta, S. *et al*, *Indian J. Chem.*, 1975, **13**, 785 (*isol, uv*)
Chhabra, S.C. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 421 (*synth, uv, ir, pmr*)
Joshi, K.C. *et al*, *J. Indian Chem. Soc.*, 1979, **56**, 327 (*isol*)
Herz, W. *et al*, *Phytochemistry*, 1982, **21**, 2683 (*isol*)
Voirin, B., *Phytochemistry*, 1983, **22**, 2107 (*uv*)
Vázquez, M.M. *et al*, *Phytochemistry*, 1988, **27**, 3706 (*isol*)

1,5-Heptanediol, 9CI H-80030

Updated Entry replacing H-00291

[60096-09-5]

$$H_3CCH_2CH(OH)CH_2CH_2CH_2CH_2OH$$

$C_7H_{16}O_2$ M 132.202

(±)-form
Liq. Insol. H_2O. d_4^{20} 0.971. Bp_{11} 135-136°. n_D^{22} 1.4571.

Pierce, J.S. *et al*, *J. Am. Chem. Soc.*, 1925, **47**, 1098.
Paul, R., *Bull. Soc. Chim. Fr.*, 1935, **2**, 311.
Bihovsky, R. *et al*, *J. Org. Chem.*, 1988, **53**, 4026 (*synth*)

3-Heptynoic acid H-80031

[59862-93-0]

$$H_3CCH_2CH_2C{\equiv}CCH_2COOH$$

$C_7H_{10}O_2$ M 126.155
Liq. Bp_{22} 140-141°.

Bigley, D.B. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1972, 592 (*synth*)

4-Heptynoic acid H-80032

[42441-83-8]

$$H_3CCH_2C{\equiv}CCH_2CH_2COOH$$

$C_7H_{10}O_2$ M 126.155
Needles (pet. ether). Mp 57-59°.

4-Bromophenacyl ester: Plates (EtOH). Mp 99-100°.

Nitrile: [18719-33-0]. *4-Heptynenitrile, 9CI.* 1-*Cyano*-3-*hexyne*
C_7H_9N M 107.155
Bp_{16} 82-83°.

Ansell, M.F. *et al*, *J. Chem. Soc. C*, 1968, 217 (*synth*)

6-Heptynoic acid H-80033

[30964-00-2]

$$HC{\equiv}C(CH_2)_4COOH$$

$C_7H_{10}O_2$ M 126.155
Liq. Bp_1 93-94°.

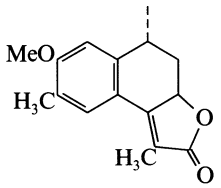
Me ester:
$C_8H_{12}O_2$ M 140.182
Bp_{11} 80°.

Nitrile: [15295-69-9]. *6-Heptynenitrile, 9CI.* 6-*Cyano*-1-*hexyne*
C_7H_9N M 107.155
Bp_{14} 87-93°.

Taylor, W.R. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 4263 (*synth*)

Ferrier, R.J. *et al*, *J. Chem. Soc.*, 1957, 1435 (*synth, nitrile*)
Gautier, J.A. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 1551 (*nitrile*)
Moody, C.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3249 (*synth, anhydride, ir, pmr, ms*)

Heritonin H-80034

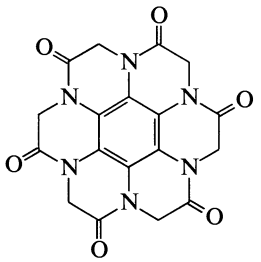


$C_{16}H_{18}O_3$ M 258.316
Isol. from *Heritiera littoralis*. Piscicide. Cryst. (C_6H_6/Et_2O). Mp 115-116°.

Miles, P.H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 896 (*isol, pmr*)

2*a*,4*a*,6*a*,8*a*,10*a*,12*a*-Hexaazacoronene-1,3,5,7,9,11(2*H*,4*H*,6*H*,8*H*,10*H*,12*H*)-hexone, 9CI H-80035

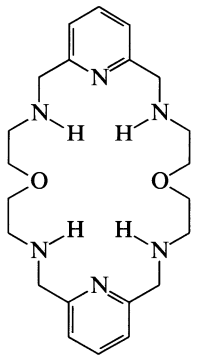
[92187-33-2]



$C_{18}H_{12}N_6O_6$ M 408.329
Fine powder. Mp >350°.

Thomaides, J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3970 (*synth, pmr, ms, ir*)

3,9,17,23,29,30-Hexaaza-6,20-dioxa-tricyclo[23.3.1.1^{11,15}]triaconta-1(28),11(29),12,14,25,27-hexaene H-80036

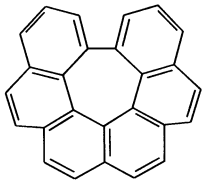


$C_{20}H_{34}N_6O_2$ M 390.528
B,HCl: V. hygroscopic solid + 2EtOH. Mp 160°.
N-*Tetrakis(4-methylbenzenesufonyl):* Cryst. (CH_2Cl_2/hexane). Mp 185°.

Hosseini, M.W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1066 (*synth*)

Hexa[7]circulene H-80037

Updated Entry replacing H-00485
*1,14-Ethenonaphtho[1′,8′:5,6,7]cyclohepta[1,2,3,4-*def*]phenanthrene, 9CI. 1,16-Didehydrohexahelicene*
[56594-61-7]



$C_{26}H_{14}$ M 326.397
Pale-yellow plates (EtOH aq.). Mp 162-163°. May be resolved chromatographically at low temp. V. optically labile.

Jessup, P.J. *et al*, *Tetrahedron Lett.*, 1975, 1453; *Aust. J. Chem.*, 1976, **29**, 173 (*synth, ms, pmr, uv*)
Yamamoto, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3578 (*resoln*)

Hexacosanal H-80038

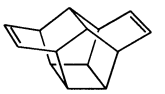
[26627-85-0]

$H_3C(CH_2)_{24}CHO$

$C_{26}H_{52}O$ M 380.696
Isol. from *Vitis vinifera* var. *sultana*. Cryst. (MeOH). Mp 73-73.5°.

Crabbé, P. *et al*, *Bull. Soc. Chim. Belg.*, 1961, **70**, 168 (*synth, ir*)
Radler, F. *et al*, *Aust. J. Chem.*, 1965, **18**, 1059 (*isol*)

Hexacyclo[6.5.1.0^{2,7}.0^{3,11}.0^{4,9}.0^{10,14}] tetradeca-5,12-diene H-80039



$C_{14}H_{14}$ M 182.265
Liq.

Chou, T.-C. *et al*, *J. Org. Chem.*, 1988, **53**, 5168 (*synth, ir, pmr, cmr, ms*)

7,9,11,13-Hexadecatetraen-1-al H-80040

[65398-27-8]

$H_3CCH_2(CH{=}CH)_4(CH_2)_5CHO$

$C_{16}H_{24}O$ M 232.365
Present in leaves of *Centaurea* spp. Not isol. in pure form.

(all-E)-form [32507-72-5]
Present in *Zoegea baldshuanica*. Not isol. in pure form.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3544; 1971, **104**, 961 (*isol, struct*)
Andersen, A.B. *et al*, *Phytochemistry*, 1977, **16**, 1829 (*isol*)

6,8,12,14-Hexadecatetraen-10-yn-1-ol, 9CI H-80041

[77319-35-8]

$H_3CCH{=}CHCH{=}CHC{\equiv}CCH{=}CHCH{=}CH(CH_2)_4CH_2OH$

$C_{16}H_{22}O$ M 230.349

(all-E)-form [1540-99-4]

Isol. from above ground parts of *Dahlia merckii*, from roots of *Bupleurum gibraltaricum*, from *Zoegea baldshuanica* and above ground parts of *Serrulata gmelini*. Shows pesticidal and herbicidal props. Needles or leaflets (pet. ether). Mp 76-77° (65-71°).

Ac: 1-Acetoxy-6,8,12,14-hexadecatetraen-10-yne
$C_{18}H_{24}O_2$ M 272.386
Isol. from *D. merckii*. Leaflets (pet. ether). Mp 52-53°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 872; 1967, **100**, 1915, 1936; 1971, **104**, 961; 1975, **108**, 2822 (*isol, uv, ir, pmr, struct, ms, synth*)
Canadian Pat., 1 172 460, (1984); *CA*, **102**, 57830z (*use*)

6,8,14-Hexadecatriene-10,12-diyn-1-al H-80042

[65398-29-0]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH{=}CH(CH_2)_4CHO$

$C_{16}H_{18}O$ M 226.318

(all-E)-form [13894-88-7]
Isol. from leaves of *Centaurea involucrata*. Oil. λ_{max} 249, 266, 296, 314, 337 nm (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3544 (*isol, struct*)
Andersen, A.B. *et al*, *Phytochemistry*, 1977, **16**, 1829 (*isol*)

1,6,8-Hexadecatriene-10,12,14-triyne H-80043

[6112-04-5]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH{=}CH(CH_2)_3CH{=}CH_2$

$C_{16}H_{16}$ M 208.302

(E,E)-form [3513-88-0]
Isol. from above-ground parts of *Chrysanthemum ircutianum* and *C. maximum*. Cryst. Mp ~20°. λ_{max} 258, 269, 288, 305, 325, 348 nm (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 2596; 1966, **99**, 586 (*isol, uv, ir, struct*)
Wrang, P.A. *et al*, *Phytochemistry*, 1975, **14**, 1027 (*isol*)

7,12,14-Hexadecatrien-10-yn-1-ol H-80044

$H_3CCH{=}CHCH{=}CHC{\equiv}CCH_2CH{=}CH(CH_2)_5CH_2OH$

$C_{16}H_{24}O$ M 232.365

(7Z,12E,14E)-form [16697-19-1]
Isol. from roots of *Dahlia merckii*.

p-*Phenylazobenzoyl:* Cryst. (pet. ether). Mp 51-51.5°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 872; 1967, **100**, 1936 (*isol, struct, synth*)
Bedford, C.T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 735 (*isol*)

5-Hexadecenoic acid, 9CI H-80045

[20057-14-1]

$H_3C(CH_2)_9CH{=}CH(CH_2)_3COOH$

$C_{16}H_{30}O_2$ M 254.412

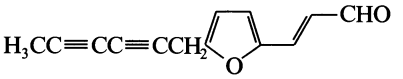
(E)-form [7056-84-0]
Isol. from seed oil of *Thalictrum venulosum*.

(Z)-form [7056-90-8]
Isol. from *T. venulosum* and *Dioscoreophyllum cumminsii* seed oils and from a strain of *Bacillus megaterium* (biosynthetically from hexadecanoic acid).

Fulco, A.J. *et al*, *J. Biol. Chem.*, 1964, **239**, 998 (*isol*)
Bhatty, M.K. *et al*, *Can. J. Biochem.*, 1966, **44**, 311 (*isol*)
Spencer, G.F. *et al*, *Lipids*, 1972, **7**, 435 (*isol*)
Starratt, A.N., *Chem. Phys. Lipids*, 1976, **16**, 215 (*synth*)

3-[5-(2,4-Hexadiynyl)-2-furanyl]-2-propenal H-80046

3-[2-(2,4-Hexadiynyl)-5-furyl]acrolein

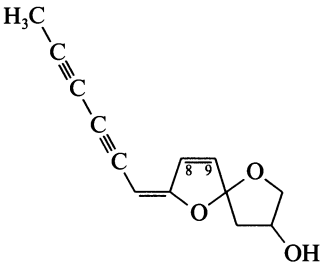


$C_{13}H_{10}O_2$ M 198.221

(E)-form
Isol. from *Chrysanthemum silvaticum*. Cryst. (Et_2O). Mp 106.5°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 2596 (*isol, uv, ir, pmr, struct, synth*)

7-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.4]non-8-en-3-ol, 9CI H-80047



(E)-form

$C_{13}H_{12}O_3$ M 216.236

(E)-form

Ac: [85799-14-0]. *8-Acetoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-3-ene*
$C_{15}H_{14}O_4$ M 258.273
Isol. from roots of *Chrysanthemum parthenium*. Cryst. (Et_2O/pet. ether). Mp 98.5°.

(Z)-form

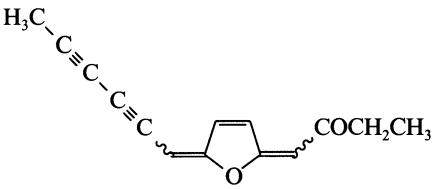
Ac: [85799-16-2].
Isol. from roots of *C. mawii*. Amorph.

Deoxy, 8,9-epoxy: ***3,4-Epoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]nonane***
$C_{13}H_{12}O_2$ M 200.237
Isol. from roots of *C. parthenifolium*. Cryst. (pet. ether). Mp 126°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1411, 2596 (*isol, uv, ir, pmr, synth*)

2-(2,4-Hexadiynylidene)-5-(propionylmethylidene)-2,5-dihydrofuran H-80048

5,8-Epoxy-4,6,8-tetradecatriene-10,12-diyn-3-one



$C_{14}H_{12}O_2$ M 212.248
Isol. from roots of *Anacyclus radiatus* and *Chrysanthemum pyrethrum*. Cryst. (pet. ether). Mp 78.5°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 588; 1964, **97**, 1179 (*isol, uv, pmr, struct*)

1,1,1,2,2,3-Hexafluoropropane, 9CI **H-80049**

[677-56-5]

$F_3CCF_2CH_2F$

$C_3H_2F_6$ M 152.039
Bp 1.2°.

[27070-61-7]

Edgell, W.F. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 4899 (*synth*)
Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1957, 2800 (*synth*)
Lelleman, D.D. *et al*, *J. Mol. Spectrosc.*, 1961, **7**, 322 (*F nmr*)

1,1,1,3,3,3-Hexafluoropropane, 9CI, 8CI **H-80050**

2,2-Dihydroperfluoropropane

[690-39-1]

$F_3CCH_2CF_3$

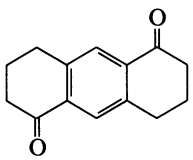
$C_3H_2F_6$ M 152.039
Shows anaesthetic props. Fp −93.62°. Bp −0.5° (0.5-1.0°)

[27070-61-7]

Tarrant, P. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 2783 (*synth*)
Lelleman, D.D. *et al*, *J. Mol. Spectrosc.*, 1961, **7**, 322 (*F nmr*)
Cheburkov, Yu.A. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1963, 1573 (*synth*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Di Paolo, T. *et al*, *J. Pharm. Sci.*, 1979, **68**, 39 (*pharmacol*)
Buerger, H. *et al*, *Spectrochim. Acta, Part A*, 1979, **35**, 517 (*ir, raman, F nmr*)
Eujen, R. *et al*, *J. Fluorine Chem.*, 1983, **22**, 263 (*F nmr*)
Bloshchitsa, F.A. *et al*, *Zh. Org. Khim.*, 1985, **21**, 1414 (*synth, F nmr, pmr*)

2,3,4,6,7,8-Hexahydro-1,5-anthracenedione, 9CI **H-80051**

[82817-91-2]

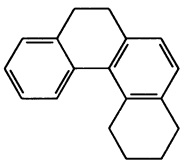


$C_{14}H_{14}O_2$ M 214.263
Cryst. (EtOAc). Mp 160°.

Caluwe, P. *et al*, *J. Org. Chem.*, 1988, **53**, 1786 (*synth, pmr, cmr*)

1,2,3,4,7,8-Hexahydrobenzo[*c*]phenanthrene, 9CI **H-80052**

[56922-96-4]



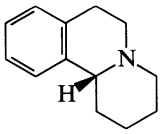
$C_{18}H_{18}$ M 234.340
Solid. Mp 77-78°. $Bp_{0.1}$ 155°.

Muller, D. *et al*, *Tetrahedron*, 1975, **31**, 1449 (*synth, ir, pmr, uv*)
Gilchrist, T.L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2595 (*synth, pmr, ms*)

1,3,4,6,7,11*b*-Hexahydro-2*H*-benzo[*a*]quinolizine **H-80053**

Benzo[a]*quinolizidine*

[55302-24-4]



(*R*)-*form*

$C_{13}H_{17}N$ M 187.284

(*R*)-*form* [2737-54-4]
Bp_7 127-128°. $[\alpha]_D$ +222° (c, 0.022 in Py).

B,HCl: [58613-60-8].
Cryst. (2-propanol). Mp 160-161°.

B,HClO$_4$: [2737-55-5].
Cryst. (2-propanol). Mp 160-161°.

B,MeI: Cryst. (2-propanol). Mp 173-174° dec.

(*S*)-*form* [17279-34-4]
Oil. $Bp_{0.03}$ 75°. $[\alpha]_D^{25}$ −206° (c, 0.017 in pyridine).
Optically pure.

B,HClO$_4$: Cryst. (2-propanol). Mp 160-162°. $[\alpha]_D$ −75.3°.

B,HCl: [17279-35-5].
$[\alpha]_D$ −140° (c, 0.425 in EtOH).

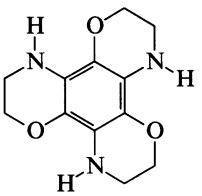
(±)-*form*

B,HCl: [20072-13-3].
Mp 242-243°.

Horii, Z. *et al*, *Tetrahedron*, 1963, **19**, 2101 (*synth, abs config, ord*)
Craig, J.C. *et al*, *Tetrahedron*, 1967, **23**, 3573 (*ord, abs config*)
Parello, J., *Bull. Soc. Chim. Fr.*, 1968, 1117 (*synth, uv*)
Meyers, A.I. *et al*, *Tetrahedron*, 1987, **43**, 5095 (*synth, ir, pmr*)

3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]oxazine, 9CI **H-80054**

[114491-24-6]



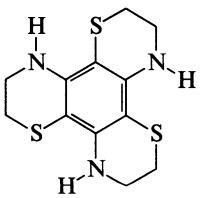
$C_{12}H_{15}N_3O_3$ M 249.269
Solid. Mp 216-219°. Mildly air sensitive.

Tri-N-*Me:* [114491-20-2].
$C_{15}H_{21}N_3O_3$ M 291.349
Solid. Mp 148-150°. Forms a cation but salts unstable.

Thomaides, J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3970 (*synth, pmr, ir, esr*)

3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]thiazine, 9CI **H-80055**

[114491-30-4]

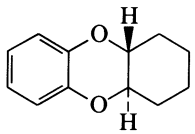


$C_{12}H_{15}N_3S_3$ M 297.469
Solid. Mp 202-204°.

Tri-N-*Me:* [114491-28-0].
$C_{15}H_{21}N_3S_3$ M 339.549
Solid. Mp 252-253°.

Thomaides, J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3970 (*synth, pmr, ir, ms, esr*)

1,2,3,4,4*a*,10*a*-Hexahydro-dibenzo[*b*,*e*][1,4]dioxin H-80056



(4*aRS*,10*aRS*)-*form*

$C_{12}H_{14}O_2$ M 190.241

(*4aRS,10aRS*)-*form* [75768-17-1]
(±)-trans-*form*
Cryst. (hexane). Mp 115-117°.

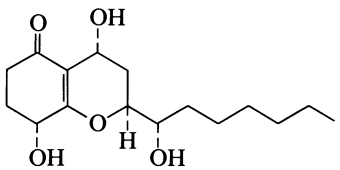
(*4aRS,10aSR*)-*form* [75459-45-9]
cis-*form*
Cryst. (MeOH). Mp 52-54° (43-44°).

Antus, S. *et al*, *Chem. Ber.*, 1989, **122**, 1017 (*synth, ir, pmr, cmr*)

2,3,4,6,7,8-Hexahydro-4,8-dihydroxy-2-(1-hydroxyheptyl)-5*H*-1-benzopyran-5-one, 9CI H-80057

4,8-Dihydroxy-2-(1-hydroxyheptyl)-3,4,5,6,7,8-hexahydro-2H-1-benzopyran-5-one

[119903-56-9]

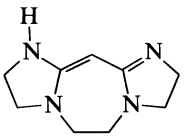


$C_{16}H_{26}O_5$ M 298.378
Metab. of *Trichoderma koningii*. Antibiotic. Needles ($CHCl_3$/pentane). Mp 122-123°. $[\alpha]_D$ +166.9° (c, 0.3 in $CHCl_3$).

Dunlop, R.W. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 67 (*isol, pmr, cmr*)

2,3,5,6,8,9-Hexahydro-1*H*-diimidazo[1,2-*d*:2′,1′-*g*][1,4]diazepine H-80058

[111062-19-2]



$C_9H_{14}N_4$ M 178.236
Readily obt. highly basic proton sponge. Mp 131-132°. pK_a 26.22 (MeCN).

B,HCl: Mp ~290° dec. Delocalised.

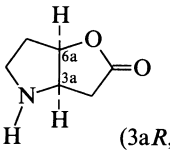
B,HClO$_4$: Mp 260-265°.

N-*Me:* [111062-21-6].
$C_{10}H_{16}N_4$ M 192.263
pK_a 26.95 (MeCN).

Schwesinger, R., *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 1164 (*synth, pmr*)

Hexahydro-2*H*-furo[3,2-*b*]pyrrol-2-one, 9CI H-80059

2-Oxa-6-azabicyclo[3.3.0]octan-3-one. 3-Hydroxypyrrolidine-2-acetic acid lactone. Geissman-Waiss lactone



(3a*R*,6a*R*)-*form*

$C_6H_9NO_2$ M 127.143
Intermed. in the synth. of retronecine and related pyrrolizidine alkaloids.

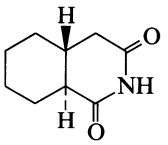
(*3aR,6aR*)-*form* [81445-21-8]
(+)-cis-*form*
B,HCl: Needles (EtOH). Mp 185-186.5°. $[\alpha]_D^{25}$ +48.8° (c, 0.20 in MeOH).

(*3aS,6aS*)-*form*
(−)-cis-*form*
B,HCl: [118710-52-4].
Mp 182-184°. $[\alpha]_D$ −42.9°.

Geissman, T.A. *et al*, *J. Org. Chem.*, 1962, **27**, 139 (*synth*)
Rueger, H. *et al*, *Heterocycles*, 1982, **19**, 23 (*synth*)
Buchanan, J.G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 2377 (*synth, ir, pmr*)
Shishido, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 993 (*synth*)
Cooper, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 509 (*synth*)

Hexahydro-1,3(2*H*,4*H*)-isoquinolinedione, 9CI H-80060

2-Carboxycyclohexaneacetic acid imide. 3-Azabicyclo[4.4.0]decane-2,4-dione



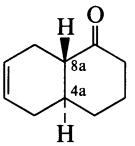
$C_9H_{13}NO_2$ M 167.207

(*4aR,8aS*)-*form* [116673-41-7]
Cryst. (toluene/hexane). Mp 186-187°. $[\alpha]_D^{20}$ −73° (c, 1.2 in $CHCl_3$).

Poloński, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 639 (*synth, uv, ir, pmr*)

3,4,4*a*,5,8,8*a*-Hexahydro-1(2*H*)-naphthalenone H-80061

Δ^6-*1-Octalone*



(4*aS*,8*aS*)-*form*

$C_{10}H_{14}O$ M 150.220

(*4aS,8aS*)-*form*
(+)-trans-*form*
Cryst. by subl. Mp 57-58°. $[\alpha]_D$ +88° (c, 0.693 in pet. ether).

(*4aRS,8aRS*)-*form* [70749-11-0]
(±)trans-*form*
Mp 46-47° (32-34°). Bp_{14} 111-112°.

Oxime:

$C_{10}H_{15}NO_2$ M 181.234
Cryst. (EtOH). Mp 154-156°.

2,4-Dinitrophenylhydrazone: [83586-08-7].
Mp 195-196°.

(4aRS,8aSR)-form [70749-10-9]
(±)-cis-*form*
Liq.

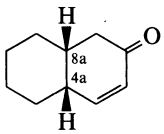
[78341-47-6]

Ireland, R.E. *et al*, *J. Org. Chem.*, 1962, **27**, 1620 (*synth*)
Acklin, W. *et al*, *Helv. Chim. Acta*, 1965, **48**, 1725 (*synth, abs config*)
Fringuelli, F. *et al*, *J. Org. Chem.*, 1982, **47**, 5056 (*synth, cmr*)
Angell, E.C. *et al*, *J. Org. Chem.*, 1988, **53**, 1424 (*synth, ir, pmr, cmr*)

4*a*,5,6,7,8,8*a*-Hexahydro-2(1*H*)-naphthalenone H-80062

Δ^3-*2-Octalone*

[2384-50-1]



(*4aRS,8aRS*)-*form*

$C_{10}H_{14}O$ M 150.220

(4aRS,8aRS)-form [55999-54-7]
(±)-cis-form
Oil. $Bp_{0.1}$ 75-77°.

(4aRS,8aSR)-form [71956-17-7]
(±)-trans-form
Liq. Bp_{12} 127-130°, $Bp_{0.1}$ 85°.

Oxime:
$C_{10}H_{15}NO$ M 165.235
Needles (Et_2O). Mp 145°.

Semicarbazone: Cryst. (EtOH aq.). Mp 188-190°.

2,4-Dinitrophenylhydrazone: Mp 194-195°.

[18317-63-0]

Lehmann, E. *et al*, *Ber.*, 1934, **67**, 1867 (*synth*)
Mühle, H. *et al*, *Helv. Chim. Acta*, 1962, **45**, 1475 (*synth, uv, ir*)
Corey, E.J. *et al*, *Tetrahedron Lett.*, 1978, 4597 (*synth*)
Angell, E.C. *et al*, *J. Org. Chem.*, 1988, **53**, 1424 (*synth, ir, pmr, cmr*)

1,2,3,9,10,10*a*-Hexahydrophenanthrene H-80063

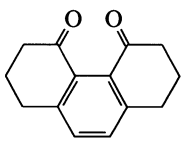
[62690-96-4]

$C_{14}H_{16}$ M 184.280
Oil.

Chini, M. *et al*, *J. Org. Chem.*, 1989, **54**, 3930 (*synth, pmr*)

1,2,3,6,7,8-Hexahydro-4,5-phenanthrenedione H-80064

[110028-98-3]

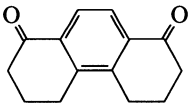


$C_{14}H_{14}O_2$ M 214.263
Cryst. (hexane). Mp 130°.

Caluwe, P. *et al*, *J. Org. Chem.*, 1988, **53**, 1786 (*synth, pmr, cmr*)

2,3,4,5,6,7-Hexahydro-1,8-phenanthrenedione, 9CI H-80065

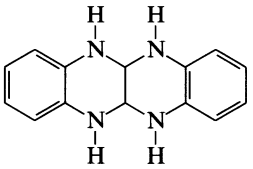
[82817-89-8]



$C_{14}H_{14}O_2$ M 214.263
Cryst. (Et_2O). Mp 167-168°.

Caluwe, P. *et al*, *J. Org. Chem.*, 1988, **53**, 1786 (*synth, ir, pmr*)

5,5*a*,6,11,11*a*,12-Hexahydroquinoxalino[2,3-*b*]quinoxaline H-80066



$C_{14}H_{14}N_4$ M 238.291

N-*Tetra-Me:* [13784-23-1].
$C_{18}H_{22}N_4$ M 294.399
Cryst. Mp 167-169°.

Tauer, E. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 338 (*synth, pmr, uv*)

3,3′,4′,5,6,7-Hexahydroxyflavone H-80067

Updated Entry replacing H-20066

Quercetagetin

[90-18-6]

$C_{15}H_{10}O_8$ M 318.239
Isol. from *Tagetes patula* (African marigold), *Gmelina arborea*, *G. asiatica*, *Artemesia taurica* and *Eriocaulon* spp. Pale-yellow cryst. + $2H_2O$ (EtOH aq.). Mp 318-320° (232-234°).

7-Glucoside: [548-75-4]. ***Quercetagitrin***
$C_{21}H_{20}O_{13}$ M 480.381
Isol. from petals of *T. erecta* (African marigold) and *Lepidophorum*, *Tetragonotheca* and *Anacyclus* spp.
Cryst. (Py aq.). Mp 236-238° dec.

3,3′-Di-Me ether: [36034-36-3]. *4′,5,6,7-Tetrahydroxy-3,3′-dimethoxyflavone*
$C_{17}H_{14}O_8$ M 346.293
Isol. from *Parthenium tomentosum*. Cryst. (C_6H_6/Me_2CO). Mp 214-215° (242-244°).

3,3′,6-Tri-Me ether:
Found in *Prunus avium*, *Fluorensia ilicitolia* and *Centaurea hyssopifolia*. Pale yellow needles. Mp 127-133°.

3,3′,6-Tri-Me ether, 7-O-β-D-glucopyranoside: [35305-11-4]. ***Jacein***
$C_{24}H_{26}O_{13}$ M 522.462
Constit. of *Centaurea jacea* and *C. hyssopifolia*. Cryst. Mp 205-207°. $[\alpha]_D^{20}$ −73.1° (c, 1.48 in MeOH).

3,3′,5,6,7-Penta Me ether: 4′-Hydroxy-3,3′,5,6,7-pentamethoxyflavone
$C_{20}H_{20}O_8$ M 388.373
Constit. of *Jasonia montana*.

3,3′,6,7-Tetra-Me ether: [603-56-5]. *4′,5-Dihydroxy-3,3′,6,7-tetramethoxyflavone*. ***Chrysosplenetin***

$C_{19}H_{18}O_8$ M 374.346
Constit. of leaves of *Plectranthus marrubioides*. Cryst. (MeOH or EtOH). Mp 182-183°.

3,3′,4′,5,6-Penta-Me ether: [57393-68-7]. *7-Hydroxy-3,3′,4′,5,6-pentamethoxyflavone*
$C_{20}H_{20}O_8$ M 388.373
Constit. of *Ambrosia grayi*. Mp 132-135°.

Hexa-Me ether: [1251-84-9]. *3,3′,4′,5,6,7-Hexamethoxyflavone. Hexamethylquercetagenin*
$C_{21}H_{22}O_8$ M 402.400
Cryst. (Me_2CO). Mp 142-143°.

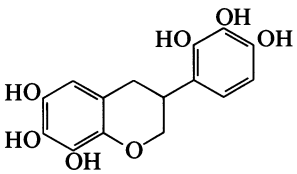
3,3′,6,7-Tetra Me ether: 4′,5-Dihydroxy-3,3′,6,7-tetramethoxyflavone
$C_{19}H_{18}O_8$ M 374.346
Constit. of *B. malcomii*. Cryst. Mp 189-191°. Originally described as 5′,6-Dihydroxy-2′,3,5,7-trimethoxyflavone.

3,3′,4′,6,7-Penta-Me ether: 5-Hydroxy-3,3′,4′,6,7-pentamethoxyflavone
$C_{20}H_{20}O_8$ M 388.373
Constit. of *B. malcomii*. Cryst. Mp 166-168°. Originally described as 6-Hydroxy-2′,3,5,5′,7-pentamethoxyflavone.

3,6,7-Tri-Me ether: 3′,4′,5-Trihydroxy-3,6,7-trimethoxyflavone
$C_{18}H_{16}O_6$ M 328.321
Constit. of *Blumea malconnii*. Cryst. (Me_2CO). Mp 252°. Originally described as 2′,5′,6-Trihydroxy-3,5,7-trimethoxyflavone.

Baker, W. *et al*, *J. Chem. Soc.*, 1929, 74 (*isol*)
Farkas, L. *et al*, *Chem. Ber.*, 1964, **97**, 610 (*isol*)
Bate-Smith, E.C. *et al*, *Phytochemistry*, 1969, **8**, 1035 (*isol*)
González, A.G. *et al*, *An. Quim.*, 1971, **67**, 795 (*isol*)
Tarpo, E., *CA*, 1971, **19**, 25 (*isol*)
Hensch, M. *et al*, *Helv. Chim. Acta*, 1972, **55**, 1610 (*deriv*)
Rodriguez, E. *et al*, *Phytochemistry*, 1972, **11**, 1507 (*isol*)
Ickes, G.R. *et al*, *J. Pharm. Sci.*, 1973, **62**, 1009 (*isol*)
Nair, A.G.R. *et al*, *Phytochemistry*, 1975, **14**, 1135 (*isol*)
Herz, W. *et al*, *Tetrahedron*, 1975, **31**, 1577 (*deriv*)
Oganesyan, E.S. *et al*, *Khim. Prir. Soedin.*, 1976, 599 (*isol*)
Wagner, H. *et al*, *Tetrahedron Lett.*, 1976, 67 (*synth*)
Bacon, J.D. *et al*, *Phytochemistry*, 1978, **17**, 1939 (*isol*)
Kiso, Y. *et al*, *Heterocycles*, 1982, **19**, 1615 (*isol*)
Kulkarni, M.M. *et al*, *Phytochemistry*, 1987, **26**, 2079 (*isol*)
Shilin, Y. *et al*, *Phytochemistry*, 1989, **28**, 1509 (*isol*)
Markham, K.R., *Phytochemistry*, 1989, **28**, 243 (*struct*)
Ahmed, A.A. *et al*, *Phytochemistry*, 1989, **28**, 665 (*isol*)

2′,3′,4′,6,7,8-Hexahydroxyisoflavan H-80068



$C_{15}H_{14}O_7$ M 306.271

3′,4′,7-Tri-Me ether: [51798-41-5]. *2′,6,8-Trihydroxy-3′,4′,7-trimethoxyisoflavan.* ***Machaerol C***
$C_{18}H_{20}O_7$ M 348.352
Isol. from heartwood of *Machaerium pedicellatum*. Tentative struct.

3′,4′,7,8-Tetra-Me ether: [51798-42-6]. *2′,6-Dihydroxy-3′,4′,7,8-tetramethoxyisoflavan.* ***Machaerol B***
$C_{19}H_{22}O_7$ M 362.379
Isol. from *M. pedicellatum* heartwood. Tentative struct.

Hexa-Me ether: 2′,3′,4′,6,7,8-Hexamethoxyisoflavan
Mp 77-79°.

Ogiyama, K. *et al*, *Phytochemistry*, 1973, **12**, 2544 (*isol, pmr*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*struct*)

2′,4′,5,5′,6,7-Hexahydroxyisoflavone H-80069

Updated Entry replacing D-20312

$C_{15}H_{10}O_8$ M 318.239

2′,4′,5′,6-Tetra-Me ether: [4935-92-6]. *5,7-Dihydroxy-2′,4′,5′,6-tetramethoxyisoflavone. 5,7-Dihydroxy-6-methoxy-3-(2,4,5-trimethoxyphenyl)-4H-1-benzopyran-4-one, 9CI.* ***Caviunin***
$C_{19}H_{18}O_8$ M 374.346
Isol. from *Dalbergia nigra* and several other *D.* spp. Needles (EtOH). Mp 191-193°.

2′,4′,5′,6-Tetra-Me ether, 7-O-glucoside: [50299-68-8].
$C_{25}H_{28}O_{13}$ M 536.488
Isol. from *D. paniculata* roots and *D. sissoo* pods. Fibrous cryst. (EtOH). Mp 236-237°.

2′,4′,5′,6-Tetra-Me ether, 7-O-rhamnosylglucoside: [75883-12-4].
$C_{31}H_{38}O_{17}$ M 682.631
Isol. from roots of *D. paniculata*. Dihydrate. Mp 138-139°.

2′,4′,5′,6-Tetra-Me ether, 7-O-gentiobioside: [72578-98-4].
$C_{31}H_{38}O_{18}$ M 698.630
Isol. from pods of *D. sissoo*. Mp 210-212°.

Farkas, L. *et al*, *Chem. Ber.*, 1961, **94**, 2501 (*synth*)
Gottlieb, O.R. *et al*, *J. Org. Chem.*, 1961, **26**, 2449 (*isol*)
Dyke, S.F. *et al*, *J. Org. Chem.*, 1961, **26**, 2453 (*synth*)
Várady, J., *Tetrahedron Lett.*, 1965, 4273 (*synth*)
Gottlieb, H.E., *Phytochemistry*, 1977, **16**, 1811 (*cmr*)
Radhakrishniah, M., *J. Indian Chem. Soc.*, 1979, **46**, 81 (*glucoside*)
Sharma, A. *et al*, *Phytochemistry*, 1979, **18**, 1253 (*gentiobioside*)
Rajulu, K.G. *et al*, *Phytochemistry*, 1980, **19**, 1563 (*rhamnosylglucoside*)

2′,4′,5,5′,7,8-Hexahydroxyisoflavone H-80070

5,7,8-Trihydroxy-3-(2,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one

$C_{15}H_{10}O_8$ M 318.239

2′,4′,5′,8-Tetra-Me ether: [4968-78-9]. *5,7-Dihydroxy-2′,4′,5′,8-tetramethoxyisoflavone.* ***Isocaviunin***
$C_{19}H_{18}O_8$ M 374.346
Isol. from pods of *Dalbergia sissoo*. Mp 193-194°.

2′,4′,5′,8-Tetra-Me ether, 7-O-glucoside: [74148-49-5]. ***Isocaviudin***
$C_{25}H_{28}O_{13}$ M 536.488
Isol from *D. sissoo* and *D. paniculata*. Cryst. (EtOH). Mp 220-222° (189-190°). $[\alpha]_D^{25}$ −30.7° (DMSO).

2′,4′,5′,8-Tetra-Me ether, 7-O-gentiobioside: [74517-73-0].
$C_{31}H_{38}O_{18}$ M 698.630
Isol. from pods of *D. sissoo*. Yellow. Mp 170-172°. $[\alpha]_D^{25}$ −65.6° (DMSO).

Sharma, A. *et al*, *Indian J. Chem., Sect. B*, 1979, **18**, 472; 1980, **19**, 237 (*isol, struct, uv, pmr, ms*)
Sharma, A. *et al*, *Phytochemistry*, 1980, **19**, 715 (*gentiobioside*)

3′,4′,5,5′,6,7-Hexahydroxyisoflavone H-80071

Updated Entry replacing T-03532

5,6,7-Trihydroxy-3-(3,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one. Irigenol

$C_{15}H_{10}O_8$ M 318.239

3′,4′,6-Tri-Me ether: [548-76-5]. *3′,5,7-Trihydroxy-4′,5′,6-trimethoxyisoflavone.* ***Irigenin***
$C_{18}H_{16}O_8$ M 360.320

Constit. of several *Iris* spp. and of *Juniperus macropoda*. Shows antifungal props. Pale-yellow needles or plates (EtOH aq.). Mp 185°.

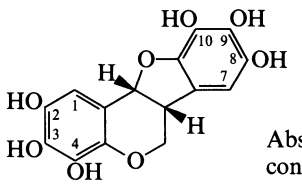
3′,4′,6-Tri-Me ether, 7-O-β-D-Glucopyranoside: [491-74-7]. ***Iridin***
$C_{24}H_{26}O_{13}$ M 522.462
From *I.* spp., *Belamcanda chinensis* and *J. macropoda*. Needles (MeOH aq.). Mp 208°.

3′,4′,5′,6-Tetra-Me ether: [78134-86-8]. *5,7-Dihydroxy-3′,4′,5′,6-tetramethoxyisoflavone.* ***Junipegenin C***
$C_{19}H_{18}O_8$ M 374.346
Isol. from leaves of *J. macropoda*. Fine needles (EtOAc). Mp 233-235°.

3′,4′,5,5′-Tetra-Me, 6,7-methylenedioxy ether: [41743-73-1]. *3′,4′,5,5′-Tetramethoxy-6,7-methylenedioxyisoflavone.* ***Irisflorentin***
$C_{20}H_{18}O_8$ M 386.357
Isol. from *I. florentina*, *I. germanica* and *I. tingitana*. Needles (MeOH). Mp 175°.

Baker, W., *J. Chem. Soc.*, 1928, 1022 (*bibl*)
Baker, W. *et al*, *J. Chem. Soc. C*, 1970, 1219 (*synth*)
Dhar, K.L. *et al*, *Phytochemistry*, 1972, 3097 (*isol*)
Arisawa, M. *et al*, *Chem. Pharm. Bull.*, 1973, **21**, 2323 (*deriv*)
Morita, N. *et al*, *Chem. Pharm. Bull.*, 1973, **21**, 600 (*Irisflorentin*)
Johnson, G. *et al*, *Physiol. Plant Pathol.*, 1976, **8**, 225 (*pharmacol*)
Sethi, M.L. *et al*, *Phytochemistry*, 1981, **20**, 341 (*Junipegenin C*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

2,3,4,8,9,10-Hexahydroxypterocarpan H-80072



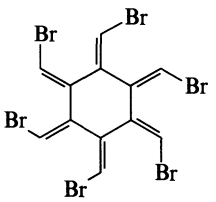
Absolute configuration

$C_{15}H_{12}O_8$ M 320.255

3,4,9,10-Tetra-Me ether: [89675-61-6]. *2,8-Dihydroxy-3,4,9,10-tetramethoxypterocarpan*
$C_{19}H_{20}O_8$ M 376.362
Isol. from *Swartzia laevicarpa* trunkwood. Cryst. (hexane). Mp 188-190°. Cas no. refers to racemate.

Braz Filho, R. *et al*, *Phytochemistry*, 1980, **19**, 2003 (*isol, uv, pmr, ord, ms, struct, abs config*)

Hexakis(bromomethylene)cyclohexane, 9CI H-80073



$C_{12}H_6Br_6$ M 629.603

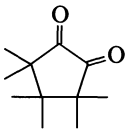
(all-E)-form
Cryst. Mp >110° slow dec.

[117965-68-1, 118099-26-6]

Shepherd, M.K., *J. Chem. Soc., Perkin Trans.* 1, 1988, 961 (*synth, pmr, cmr, ms*)

3,3,4,4,5,5-Hexamethyl-1,2-cyclopentanedione H-80074

[16980-19-1]



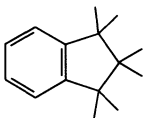
$C_{11}H_{18}O_2$ M 182.262
Orange cryst. solid. Mp 105-110°.

Crandall, J.K. *et al*, *J. Org. Chem.*, 1968, **33**, 3291 (*synth, ir, uv, pmr*)
Baran, J. *et al*, *J. Org. Chem.*, 1988, **53**, 4626 (*synth*)

1,1,2,2,3,3-Hexamethylindane H-80075

*2,3-Dihydro-1,1,2,2,3,3-hexamethyl-1*H*-indene*

[91324-94-6]



$C_{15}H_{22}$ M 202.339
Liq. $Bp_{0.38}$ 52-55°.

Baran, J. *et al*, *J. Org. Chem.*, 1988, **53**, 4626 (*synth, ir, pmr, cmr, ms*)

Hexamethylpentanedioic acid, 9CI H-80076

Hexamethylglutaric acid

[115942-55-7]

$$HOOCC(CH_3)_2C(CH_3)_2C(CH_3)_2COOH$$

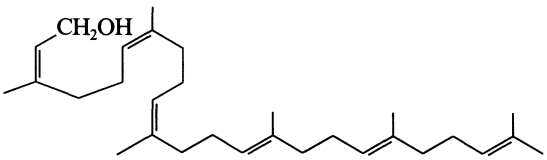
$C_{11}H_{20}O_4$ M 216.277
Cryst. (MeOH). Mp 188-189° dec.

Di-Me ester: [115942-56-8].
$C_{13}H_{24}O_4$ M 244.330
Viscous liq. $Bp_{0.42}$ 90° (bath) .

Anhydride: [115942-54-6]. *Dihydro-3,3,4,4,5,5-hexamethyl-2*H*-pyran-2,6(3*H*)dione, 9CI*
$C_{11}H_{18}O_3$ M 198.261
Cryst. by subl. Mp 174-175°.

Baran, J. *et al*, *J. Org. Chem.*, 1988, **53**, 4626 (*synth, ir, pmr, cmr*)

3,7,11,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaen-1-ol H-80077



$C_{30}H_{50}O$ M 426.724

(2Z,6Z,10Z,14E,18E,22E)-form
Constit. of *Phyllanthus niruri*. Viscous mass.

Moiseenkov, A.M. *et al*, *Tetrahedron Lett.*, 1981, **22**, 3309 (*synth*)
Singh, B. *et al*, *Phytochemistry*, 1989, **28**, 1980 (*isol*)

5-Hexen-1-amine, 9CI H-80078

6-Amino-1-hexene

[34825-70-2]

$$H_2C{=}CHCH_2CH_2CH_2CH_2NH_2$$

$C_6H_{13}N$ M 99.175
Liq. Bp 130-132°, Bp_{55} 58°.
Phenylthiourea deriv.: Cryst. (EtOAc/pet. ether or EtOH). Mp 57°.
N-*Me:*
$C_7H_{15}N$ M 113.202
Bp_{750} 129-130°. n_D^{25} 1.4229.

Cogdell, T.J., *J. Org. Chem.*, 1972, **37**, 2541 (*synth, pmr*)
Abd El Samii, Z.K.M. *et al, J. Chem. Soc., Perkin Trans.* 1, 1988, 2517 (*synth*)

2-Hexenedial H-80079

[4216-41-5]

$OHCCH_2CH_2CH{=}CHCHO$

$C_6H_8O_2$ M 112.128
(Z)-form
$Bp_{0.35}$ 60° (Kugelrohr) .

Hudlicky, T. *et al, J. Am. Chem. Soc.*, 1988, **110**, 4735 (*synth, pmr, ir, ms*)

3-Hexenedial H-80080

[6820-21-9]

$OHCCH_2CH{=}CHCH_2CHO$

$C_6H_8O_2$ M 112.128
[72530-32-6]

Uchida, M. *et al, Agric. Biol. Chem.*, 1979, **43**, 1919 (*synth, ir*)

2-Hexene-1,6-diol H-80081

$HOCH_2CH{=}CHCH_2CH_2CH_2OH$

$C_6H_{12}O_2$ M 116.160
(E)-form [63974-05-0]
$Bp_{0.01}$ 100-105°.
(Z)-form [38796-35-9]
$Bp_{0.3}$ 96°.

Paquette, L.A. *et al, J. Am. Chem. Soc.*, 1972, **94**, 6751 (*synth, pmr, ir*)
Egmond, G.J.N. *et al, Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1977, **96**, 172 (*synth, pmr, ir*)

3-Hexene-1,6-diol H-80082

[67077-43-4]

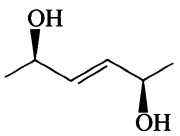
$HOH_2CCH_2CH{=}CHCH_2CH_2OH$

$C_6H_{12}O_2$ M 116.160
(Z)-form [72530-33-7]
$Bp_{0.6}$ 105-110°.
[71655-17-9]

Uchida, M. *et al, Agric. Biol. Chem.*, 1979, **43**, 1919 (*synth, ir, pmr, ms*)

3-Hexene-2,5-diol, 9CI H-80083

Updated Entry replacing H-00862
[7319-23-5]



(2RS,5RS)-(E)-form

$C_6H_{12}O_2$ M 116.160

(2RS,5RS)-(E)-form
(±)-trans-*form*
Cryst. (Et_2O). Mp 97°.
Di-Me ether: [98721-08-5]. *2,5-Dimethoxy-3-hexene*
$C_8H_{16}O_2$ M 144.213
Slightly yellow oil. Bp_{2-3} 110°.
Di-Et ether: [116910-25-9]. *2,5-Diethoxy-3-hexene*
$C_{10}H_{20}O_2$ M 172.267
Slightly yellow oil. Bp_{2-3} 125°.
(2RS,5SR)-(E)-form
meso-trans-*form*
Di-Me ether: [98721-09-6].
Oil. Bp_{2-3} 105° (kugelrohr) .
Di-Et ether: [116910-26-0].
Oil. Bp_{2-3} 110° (kugelrohr) . Cont. 15% (±)-form.
(Z)-form
Di-Ac:
$C_{10}H_{16}O_4$ M 200.234
Bp_{12} 102°. *meso-* and (±)- stereoisomers not differentiated.

Alder, K. *et al, Justus Liebigs Ann. Chem.*, 1957, **608**, 195 (*synth*)
Bäckvall, J.-E. *et al, J. Org. Chem.*, 1988, **53**, 5695 (*ether, synth, pmr, cmr, ir*)

3-Hexene-2,5-dione, 9CI H-80084

Updated Entry replacing H-00863
1,2-Diacetylethylene
[4436-75-3]

$H_3CCOCH{=}CHCOCH_3$

$C_6H_8O_2$ M 112.128
(E)-form
Pale-yellow or colourless cryst. (pet. ether). Mp 77°. Bp_{15} 90°.
Bis-2,4-dinitrophenylhydrazone: Red needles (Py). Mp 291-292°.
(Z)-form [17559-81-8]
Pale-yellow liq. Isom. to (*E*)-form after several weeks at 0°.

Goldberg, M.W. *et al, Helv. Chim. Acta*, 1938, **21**, 1699 (*synth*)
Bestman, H.-J. *et al, Chem. Ber.*, 1969, **102**, 2259 (*synth*)
Severin, T. *et al, Chem. Ber.*, 1975, **108** (*synth*)
Williams, P.D. *et al, J. Org. Chem.*, 1981, **46**, 4143 (*Z*-form)
Lepage, L. *et al, Synthesis*, 1983, 1018 (*synth*)

2-Hexyne-1,6-diol H-80085

[32114-34-4]

$HOCH_2CH_2CH_2C{\equiv}CCH_2OH$

$C_6H_{10}O_2$ M 114.144
Bp_4 145-147°, $Bp_{0.3}$ 103°.

Paquette, L.A. *et al, J. Am. Chem. Soc.*, 1972, **94**, 6751 (*synth, pmr, ir*)

5-Hexynoic acid H-80086

Updated Entry replacing H-40084
[53293-00-8]

$HC{\equiv}C(CH_2)_3COOH$

$C_6H_8O_2$ M 112.128
Liq. Bp_{20} 120-125°, Bp_6 95-96°. Claimed in one paper to be cryst., Mp 41-43.5°.
Me ester: [77758-51-1].
$C_7H_{10}O_2$ M 126.155
Bp_{10} 56°.

Chloride: [55183-45-4].
C_6H_7ClO M 130.573
Liq. $Bp_{0.5}$ 50-55°.

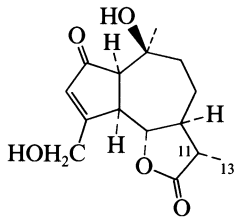
Nitrile: [14918-21-9]. *5-Cyano-1-pentyne*
C_6H_7N M 93.128
Bp_7 65.5°.

Anhydride:
$C_{12}H_{14}O_3$ M 206.241
Liq. $Bp_{0.6}$ 122-124°.

Eglington, G. *et al*, *J. Chem. Soc.*, 1953, 3052 (*synth*)
Just, G. *et al*, *Synth. Commun.*, 1979, **9**, 613 (*synth*)
Gerlach, H. *et al*, *Helv. Chim. Acta*, 1980, **63**, 2312 (*synth, pmr, ir, ms*)
Krafft, G.A. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 5459 (*synth, pmr*)
Millar, J.G. *et al*, *J. Org. Chem.*, 1984, **49**, 2332 (*synth, pmr, ms*)
Earl, R.A. *et al*, *J. Org. Chem.*, 1984, **49**, 4786 (*synth*)
Atkinson, R.S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1986, 1215 (*synth*)
Moody, C.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3249 (*anhydride*)

Hieracin I — H-80087

[117259-18-4]

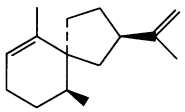


$C_{15}H_{20}O_5$ M 280.320
Constit. of *Picris hieracioides*.

11,13-Didehydro: [117259-19-5]. ***Hieracin* II**
$C_{15}H_{18}O_5$ M 278.304
Constit. of *P. hieracioides*.

Kanayama, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 2971.

Hinesene — H-80088

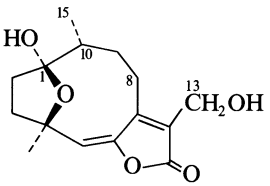


$C_{15}H_{24}$ M 204.355
Constit. of *Rolandra fruticosa*. Oil. $[\alpha]_D^{24}$ −44° (c, 0.1 in $CHCl_3$).

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1937.

Hirsutinolide — H-80089

Updated Entry replacing D-00512
[68024-72-6]



$C_{15}H_{20}O_5$ M 280.320
Parent compd. not known.

10β-Hydroxy-8β-acetoxy, 13-Ac: [72712-41-5]. *8β-Acetoxy-10β-hydroxyhirsutinolide* 13-O-*acetate*. *Hirsutolide*
$C_{19}H_{24}O_9$ M 396.393
Constit. of *Vernonia saltensis*. Oil. $[\alpha]_D^{24}$ +36.3° (c, 4.1 in $CHCl_3$). Identity of the two samples not certain.

10β-Hydroxy, 8β-acetoxy, 1,13-di-Ac: [72712-42-6]. *8β-Acetoxy-10β-hydroxyhirsutinolide* 1,13-O-*diacetate*
$C_{21}H_{26}O_{10}$ M 438.430
Constit. of *V. saltensis*. Oil. $[\alpha]_D$ −3° (c, 0.6 in $CHCl_3$).

10β-Hydroxy, 8β-propanoyloxy, 13-Ac: [71305-86-7]. *8β-Propionyloxy-10β-hydroxyhirsutinolide*-13-O-*acetate*
$C_{20}H_{26}O_9$ M 410.420
Constit. of *V. scorpioides*. Oil. $[\alpha]_D^{24}$ +63.5° (c, 0.5 in $CHCl_3$).

10β-Hydroxy, 8β-propanoyloxy, 1,13-di-Ac: [79081-71-3]. *8β-Propionyloxy-10β-hydroxyhirsutinolide* 1,13-*di*-O-*acetate*
$C_{22}H_{28}O_{10}$ M 452.457
Constit. of *V. scorpioides*. Oil.

10β-Hydroxy, 8-propanoyloxy, O¹-Me, 13-Ac: [71305-76-5]. *8-Propionoyloxy-10β-hydroxy*-1-O-*methylhirsutinolide*-13-O-*acetate*
$C_{21}H_{28}O_9$ M 424.447
Constit. of *V. scorpioides*. Oil. C8-config. uncertain.

8β,10β-Diacetoxy, 13-Ac: [72748-29-9]. *8β,10β-Diacetoxyhirsutinolide* 13-O-*acetate*
$C_{21}H_{26}O_{10}$ M 438.430
Constit. of *Stokesia laevis*. Oil. Occurs with the 1-epimer.

8β,10β-Diacetoxy, O¹-Me, 13-Ac: [72778-10-0]. *8β,10β-Diacetoxy*-1-O-*methylhirsutinolide* 13-O-*acetate*
$C_{22}H_{28}O_{10}$ M 452.457
Constit. of *S. laevis*. Oil. Occurs with the 1-epimer.

8β-(2-Methylpropenoyloxy): 8β-(2-Methylacryloxyloxy)hirsutinolide
$C_{19}H_{24}O_7$ M 364.394
Isol. from *V.* spp. Cryst. (Et_2O/pet. ether). Mp 184°. $[\alpha]_D^{24}$ −6.9° (c, 1.1 in $CHCl_3$).

8β-(2,3-Epoxy-2-methylpropanoyloxy): 8β-(2-Methyl-2,3-epoxypropionyloxy)hirsutinolide
$C_{19}H_{24}O_8$ M 380.394
Isol. from *V.* spp. Cryst. (Et_2O/pet. ether). Mp 170°. $[\alpha]_D^{24}$ +0.7° (c, 1.1 in $CHCl_3$).

8β-(2-Hydroxymethylpropenoyloxy), 13-Ac: 8β-(2-Hydroxymethylacryloyloxy)hisutinolide 13-O-*acetate*
$C_{21}H_{26}O_9$ M 422.431
Constit. of *V.* spp. Cryst. (Et_2O/pet. ether). Mp 72°. $[\alpha]_D^{24}$ +111.2° (c, 1.3 in $CHCl_3$).

8β-(2-Hydroxymethylpropenoyloxy), 15-hydroxy, 13-Ac: 8β-(2-Methylacryloyloxy)-15-hydroxyhisutinolide 13-*acetate*
$C_{21}H_{26}O_9$ M 422.431
Isol. from *V.* spp. Oil. Misnamed in the paper.

8β-(2-Methylpropenoyloxy), 13-Ac: 8β-(2-Methylacryloyloxy)hirsutinolide 13-O-*acetate*
$C_{21}H_{26}O_8$ M 406.432
Isol. from *V.* spp. Oil. $[\alpha]_D^{24}$ +19.5° (c, 1.0 in $CHCl_3$).

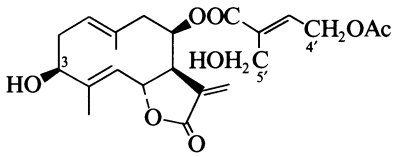
8β-(2,3-Epoxy-2-methylpropanoyloxy), 13-Ac: 8β-(2-Methyl-2,3-epoxypropionyloxy)hirsutinolide 13-O-*acetate*
$C_{21}H_{26}O_9$ M 422.431
Isol. from *V.* spp. Oil. $[\alpha]_D^{24}$ +18.3° (c, 2.05 in $CHCl_3$).

Bohlmann, F. *et al*, *Phytochemistry*, 1978, **17**, 475; 1979, **18**, 289, 987 (*isol, pmr*)
Rustaiyan, A.N. *et al*, *Fitoterapia*, 1979, **50**, 243 (*Hirsutolide*)

Hiyodorilactone D H-80090

Updated Entry replacing H-00999

[72493-40-4]



$C_{22}H_{28}O_8$ M 420.458

Constit. of *Eupatorium sachalinense*. Yellow oil. $[\alpha]_D^{28}$ +81° (c, 0.36 in EtOH).

4′-Deacetyl, 5′-Ac: [72493-41-5]. ***Hiyodorilactone E.*** *Santhemoidin C*

$C_{22}H_{28}O_8$ M 420.458

Constit. of *E. sachalinense* and of *Schkuhria anthemoidea*. Cryst. Mp 149° dec., Mp 169-172°. $[\alpha]_D^{18}$ +119° (c, 0.22 in EtOH)(+75°). Hiyodorilactone E and Santhemoidin C have not been compared and their recorded props. are different.

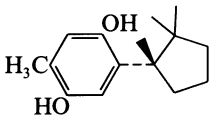
3,5′-Di-Ac: [72493-42-6]. ***Hiyodorilactone F***

$C_{26}H_{32}O_{10}$ M 504.533

Constit. of *E. sachalinense*. Yellow oil. $[\alpha]_D^{30}$ −141° (c, 0.21 in EtOH).

Takahashi, T. *et al*, *Chem. Pharm. Bull.*, 1979, **27**, 2539 (*isol*)
Pérez, A.L. *et al*, *Phytochemistry*, 1984, **23**, 2399 (*isol*)

HM-1 H-80091

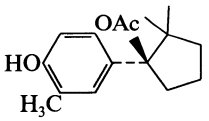


$C_{15}H_{22}O_2$ M 234.338

Metab. of fungus *Helicobasidium mompa*. Needles. Mp 139.5-140.0°. $[\alpha]_D$ −55.0° ($CHCl_3$).

Kajimoto, T. *et al*, *Chem. Lett.*, 1989, 527.

HM-2 H-80092

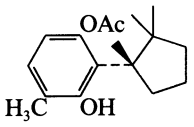


$C_{17}H_{24}O_3$ M 276.375

Metab. of *Helicobasidium mompa*. Oil. $[\alpha]_D$ −37.0° ($CHCl_3$).

Kajimoto, T. *et al*, *Chem. Lett.*, 1989, 527.

HM-3 H-80093

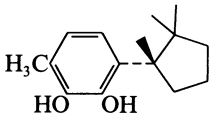


$C_{17}H_{24}O_3$ M 276.375

Metab. of *Helicobasidium mompa*. Needles. Mp 158.5-160.0°. $[\alpha]_D$ −8.1° ($CHCl_3$).

Kajimoto, T. *et al*, *Chem. Lett.*, 1989, 527.

HM-4 H-80094

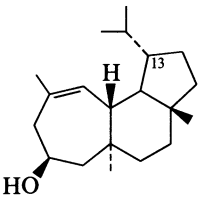


$C_{15}H_{22}O_2$ M 234.338

Metab. of *Helicobasidium mompa*. Needles. Mp 72.0-73.0°. $[\alpha]_D$ −57.4° ($CHCl_3$).

Kajimoto, T. *et al*, *Chem. Lett.*, 1989, 527.

5-Homoverrucosanol H-80095



$C_{20}H_{34}O$ M 290.488

5β-form

Constit. of *Schistochila rigidula*.

13-Epimer: [119242-42-1]. ***13-Epihomoverrucosan-5β-ol***

Constit. of *S. nobilis*. Cryst. Mp 123-124°. $[\alpha]_D$ +47.1° (c, 0.55 in $CHCl_3$).

Asakawa, Y. *et al*, *Phytochemistry*, 1988, **27**, 3509.

16,22-Hopanediol H-80096

$C_{30}H_{52}O_2$ M 444.740

16β-form

6-*Desoxyleucotylin*

Constit. of *Parmelia entotheiochroa*. Cryst. Mp 268°. $[\alpha]_D$ +68° ($CHCl_3$).

16-Ac:

$C_{32}H_{54}O_3$ M 486.777

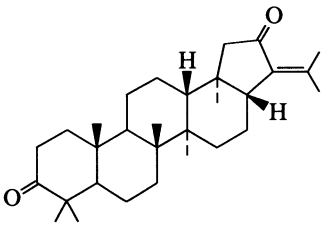
Constit. of *P. entotheiochroa*. Cryst. Mp 228°. $[\alpha]_D$ +52° ($CHCl_3$).

Yosioka, I. *et al*, *Chem. Pharm. Bull.*, 1966, **14**, 804.

21-Hopene-3,20-dione H-80097

Lageflorin

[119403-28-0]



$C_{30}H_{46}O_2$ M 438.692

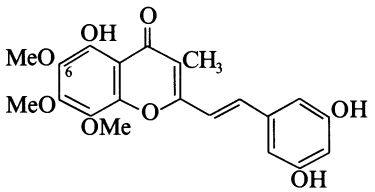
Constit. of *Lagerstroemia parviflora*. Needles (C_6H_6/pet. ether). Mp 346-348°.

Barik, B.R. *et al*, *Phytochemistry*, 1988, **27**, 3679.

Hormothamnione H-80098

Updated Entry replacing H-50127

[103654-49-5]



$C_{21}H_{20}O_8$ M 400.384

Constit. of the alga *Chrysophaeum taylori*. Potent cytotoxin. Yellow solid. Mp 270° dec.

6-Demethoxy: ***6-Desmethoxyhormothamnione***

$C_{20}H_{18}O_7$ M 370.358

Constit. of *C. taylori*. Cytotoxic agent.

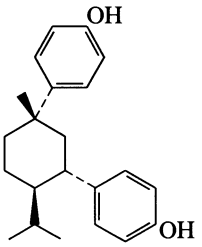
6-Demethoxy, tri-Ac: Cryst. Mp 184-186°.

Gerwick, W.H. *et al*, *Tetrahedron Lett.*, 1986, **27**, 1979 (*cryst struct*)

Gerwick, W.H., *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 252 (*isol, deriv*)

Hydrallmanol A H-80099

[121079-02-5]



$C_{22}H_{28}O_2$ M 324.462

Metab. of *Hydrallmania falcata*. Cytotoxic agent. Pale yellow oil.

Pathirana, C. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1487.

Hydrobenzamide H-80100

*1-Phenyl-*N,N′*-bis(phenylmethylene)methanediamine, 9CI.*
N,N′-Dibenzylidenetoluene-α,α-diamine, 8CI

[92-29-5]

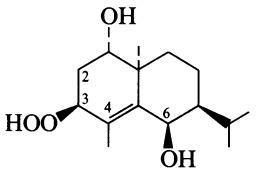
$(PhCH{=}N)_2CHPh$

$C_{21}H_{18}N_2$ M 298.387

Prisms (EtOH). Mp 107-108° (101-102°).

Sadtler Standard Infrared Spectra, No. 20378 (*ir*)
Pirrone, F., *Gazz. Chim. Ital.*, 1937, **67**, 529 (*synth*)
Ogata, Y. *et al*, *J. Org. Chem.*, 1964, **29**, 1985 (*synth*)
Nicholson, I. *et al*, *J. Chem. Soc.*, 1965, 3067 (*uv*)
Hunter, D.H. *et al*, *Can. J. Chem.*, 1972, **50**, 669 (*tautom*)
Nishiyama, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 609 (*synth, pmr*)

3-Hydroperoxy-4-eudesmene-1,6-diol H-80101



$C_{15}H_{26}O_4$ M 270.368

(1α,3β,5β,6β,10α)-form

6-Cinnamoyl: [119364-25-9]. *6β-Cinnamoyloxy-3β-hydroperoxy-5,10-bisepi-4-eudesmen-1α-ol*

$C_{24}H_{32}O_5$ M 400.514

Constit. of *Ambrosia artemisioides*. Oil.

3-Ketone, 6-cinnamoyl: [119285-46-0]. *6β-Cinnamoyloxy-1α-hydroxy-5,10-bisepi-4-eudesmen-3-one*

$C_{24}H_{30}O_4$ M 382.499

Constit. of *A. artemisioides*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551.

4-Hydroperoxy-2-eudesmene-1,6-diol H-80102

$C_{15}H_{26}O_4$ M 270.368

(1α,4β,5β,6β,10α)-form

6-Cinnamoyl: [119285-45-9]. *6β-Cinnamoyloxy-4β-hydroperoxy-5,10-bisepi-2-eudesmen-1α-ol*

$C_{24}H_{32}O_5$ M 400.514

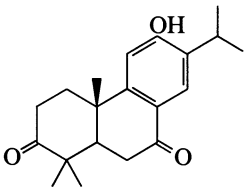
Constit. of *Ambrosia artemisioides*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551.

12-Hydroxy-8,11,13-abietatriene-3,7-dione H-80103

Nimosone

[61494-73-3]



$C_{20}H_{26}O_3$ M 314.424

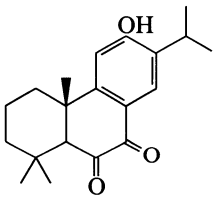
Constit. of *Azadirachta indica*. Needles ($CHCl_3$). Mp 72-73°.

Ara, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1054 (*isol, pmr, cmr*)

12-Hydroxy-8,11,13-abietatriene-6,7-dione H-80104

Hypargenin C

[119817-27-5]



$C_{20}H_{26}O_3$ M 314.424

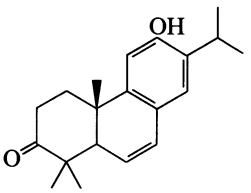
Constit. of *Salvia hypargeia*. Antibacterial agent. Orange amorph. solid.

Ulubelen, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1178 (*isol, pmr, cmr*)

12-Hydroxy-6,8,11,13-abietatrien-3-one H-80105

Hypargenin D

[119767-14-5]

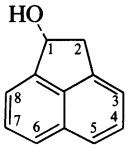


$C_{20}H_{26}O_2$ M 298.424
Constit. of *Salvia hypargeia*. Antibacterial agent. Orange amorph. solid.

Ulubelen, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1178 (*isol, pmr, cmr*)

1-Hydroxyacenaphthene H-80106

Updated Entry replacing H-01162
1,2-Dihydro-1-acenaphthylenol, 9CI. 1-Acenaphthenol, 8CI
[6306-07-6]



(*R*)-*form*

$C_{12}H_{10}O$ M 170.210

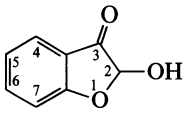
(R)-form
Mp 127-127.5°. $[\alpha]_D$ −1.46° (c, 1.23 in $CHCl_3$).

(±)-form
Needles (EtOH or C_6H_6). Mp 148° (144.5-145.5°).

Cason, J. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 432 (*synth*)
Org. Synth., 1941, **21**, 1 (*synth*)
Pratt, E.F. *et al*, *J. Org. Chem.*, 1961, **26**, 2973 (*synth*)
Gupta, M.P. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 7 (*cryst struct*)
Hu, Y. *et al*, *Can. J. Chem.*, 1989, **67**, 60 (*resoln, cryst struct, abs config*)

2-Hydroxy-3(2*H*)-benzofuranone, 9CI, 8CI H-80107

2-Hydroxy-3-coumaranone. 2,3-Dihydro-2-hydroxybenzo[b]*furan-3-one*
[17392-15-3]



$C_8H_6O_3$ M 150.134
Prisms (Et_2O). Mp 108°.

Me ether: [75335-07-8]. *2-Methoxy-3*(2H)*-benzofuranone, 9CI*
$C_9H_8O_3$ M 164.160
Oil.

Howe, R. *et al*, *J. Chem. Soc. C*, 1967, 2510 (*synth, pmr*)
Donnelly, J.A. *et al*, *Tetrahedron*, 1973, **29**, 3979 (*uv*)
Malaitong, M. *et al*, *Chem. Lett.*, 1980, 305 (*deriv*)
Antus, S. *et al*, *Justus Liebigs Ann. Chem.*, 1980, 1271 (*synth, pmr, deriv*)

4-Hydroxy-3(2*H*)-benzofuranone, 9CI, 8CI H-80108

4-Hydroxy-3-coumaranone
[19278-81-0]
$C_8H_6O_3$ M 150.134
Cryst. (C_6H_6). Mp 120° (subl. at 85°).

Me ether: 4-Methoxy-3(2H)*-benzofuranone*
$C_9H_8O_3$ M 164.160
Cryst. (C_6H_6). Mp 151°.

Et ether: 4-Ethoxy-3(2H)*-benzofuranone*
$C_{10}H_{10}O_3$ M 178.187
Cryst. (EtOH). Mp 96°.

Shriner, R.L. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 2328 (*synth*)
Farmer, V.C. *et al*, *J. Chem. Soc.*, 1956, 3600 (*deriv*)
Dallacker, F. *et al*, *Justus Liebigs Ann. Chem.*, 1966, **694**, 98 (*derivs*)
Schenck, G. *et al*, *Tetrahedron Lett.*, 1968, 2375 (*uv*)
Huke, M. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1969, **302**, 401; **302**, 423 (*uv, pmr*)

5-Hydroxy-3(2*H*)-benzofuranone, 9CI, 8CI H-80109

5-Hydroxy-3-coumaranone
[19278-82-1]
$C_8H_6O_3$ M 150.134
Yellow prisms (diisopropyl ether). Mp 152-153°.

Ac:
$C_{10}H_8O_4$ M 192.171
Plates (Et_2O/pet. ether). Mp 95-96°.

Me ether: [39581-55-0]. *5-Methoxy-3*(2H)*-benzofuranone*
$C_9H_8O_3$ M 164.160
Cryst. (MeOH). Mp 88.5-90°.

Kloetzel, M.K. *et al*, *J. Org. Chem.*, 1955, **20**, 38 (*synth, derivs*)
Schenck, G. *et al*, *Tetrahedron Lett.*, 1968, 2375 (*uv*)
Huke, M. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1969, **302**, 423 (*pmr, uv*)

6-Hydroxy-3(2*H*)-benzofuranone, 9CI, 8CI H-80110

6-Hydroxy-3-coumaranone
[6272-26-0]
$C_8H_6O_3$ M 150.134
Yellow plates (EtOH). Mp 245° dec.

Ac:
$C_{10}H_8O_4$ M 192.171
Pale yellow cryst. (EtOH). Mp 125-126°. $Bp_{0.5}$ 110° subl.

Me ether: [15832-09-4]. *6-Methoxy-3*(2H)*-benzofuranone*
$C_9H_8O_3$ M 164.160
Yellow needles (EtOH) or rose red cryst. (MeOH). Mp 124-125° (yellow form), Mp 170-171° (red form). The 2 variants are reported in different refs. and may be polymorphs, or one may be spurious.

Barltrop, J.A., *J. Chem. Soc.*, 1946, 958 (*deriv*)
Horning, E.C. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 3619 (*synth*)
Davies, J.S.H. *et al*, *J. Chem. Soc.*, 1950, 3206 (*synth*)
Dawkins, A.W. *et al*, *J. Chem. Soc.*, 1959, 2203 (*deriv*)
Logemann, W., *Chem. Ber.*, 1963, **96**, 1680 (*synth, ir*)
Doifode, K.B. *et al*, *J. Org. Chem.*, 1964, **29**, 2025 (*deriv*)
Schenck, G. *et al*, *Tetrahedron Lett.*, 1967, 2059 (*uv*)
Huke, M. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1969, **302**, 423 (*pmr, uv*)

7-Hydroxy-3(2*H*)-benzofuranone, 9CI, 8CI H-80111

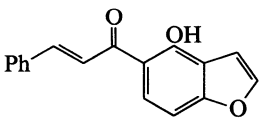
7-Hydroxy-3-coumaranone
[19397-70-7]
$C_8H_6O_3$ M 150.134
Needles (subl. at 125°). Mp 186-188° dec.

Me ether: [7169-37-1]. *7-Methoxy-3*(2H)*-benzofuranone*
$C_9H_8O_3$ M 164.160
Cryst. (Et_2O). Mp 83-84°.

Mosimann, W. *et al*, *Chem. Ber.*, 1916, **49**, 1261 (*synth*)
Richtzenhain, H. *et al*, *Ber.*, 1956, **89**, 378 (*synth, deriv*)
Schenck, G. *et al*, *Tetrahedron Lett.*, 1968, 2375 (*synth, uv*)
Jung, M.E. *et al*, *J. Org. Chem.*, 1988, **53**, 423 (*synth, ir, ms, pmr*)

1-(4-Hydroxy-5-benzofuranyl)-3-phenyl-2-propen-1-one H-80112

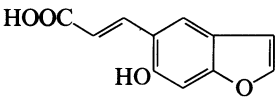
Updated Entry replacing H-70107
5-Cinnamoyl-4-hydroxybenzofuran



$C_{17}H_{12}O_3$ M 264.280
Constit. of *Milletia ovalifolia*. Yellow needles (EtOH). Mp 124°.

Saxena, D.B. *et al*, *Indian J. Chem.*, *Sect. B*, 1987, **26**, 704.

3-(6-Hydroxy-5-benzofuranyl)-2-propenoic acid H-80113



$C_{11}H_8O_4$ M 204.182

(E)-form

Furocoumaric acid. Psoralic acid
Mp 221°.

O-*β-D-Glucopyranoside:* Obt. by isom. of the natural (*Z*)-isomer in hot H_2O. Mp 244°. $[\alpha]_D^{20}$ −80.0° (H_2O).

Me ether: Mp 222°.

(Z)-form

Furocoumarinic acid
Free acid cyclises to psoralen.

O-*β-D-Glucopyranoside:*
$C_{17}H_{18}O_9$ M 366.324
Isol. from seeds of *Coronilla* spp. Biogenetic precursor to psoralen. Mp 125°. $[\alpha]_D^{20}$ −61.3° (H_2O).

Me ether: Mp 166°.

Stoll, A. *et al*, *Helv. Chim. Acta*, 1950, **33**, 1637.

4-Hydroxybenzyl alcohol H-80114

Updated Entry replacing H-01352

4-Hydroxybenzenemethanol, 9CI. α,4-Dihydroxytoluene. p-*Hydroxymethylphenol*

[623-05-2]

$C_7H_8O_2$ M 124.139
Constit. of muskmelon (*Cucurbita moschata*) seedlings and from infected bulbs of *Orchis militaris* and *Loroglossum hircinum*. Cofactor for indoleacetic acid oxidase. Prisms or needles (H_2O). Mp 124.5-125.5°.

α-Ac:
$C_9H_{10}O_3$ M 166.176
Needles (H_2O). Mp 84°.

Di-Ac: [2937-64-6].
$C_{11}H_{12}O_4$ M 208.213
Needles. Mp 75°. Bp_{11} 155-157°.

4-Me ether: [105-13-5]. *4-Methoxybenzyl alcohol. Anisyl alcohol*
$C_8H_{10}O_2$ M 138.166
Simple esters are used in flavouring. d_4^{20} 1.115. Mp 24-25°, Mp 45°. Bp_{12} 135-136°.
▷ Mod. toxic. DO8925000.

4-Me ether, Ac: [104-21-2]. *Anisyl acetate*
$C_{10}H_{12}O_3$ M 180.203
Used in flavour industry. Mp 84°. Bp_{12} 135-136°.

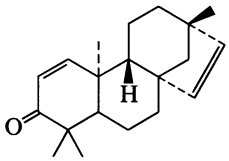
1′-Me ether: 4-(Methoxymethyl)phenol. p-*Hydroxybenzyl methyl ether*
$C_8H_{10}O_2$ M 138.166
Isol. from unripe fruits of *Citrullus colocynthis*. Plates. Mp 85-86°.

Di-Me ether: [1515-81-7].
$C_9H_{12}O_2$ M 152.193
Bp 225-226°.

Späth, E., *Monatsh. Chem.*, 1914, **35**, 319 (*synth*)
Carothers, W.H. *et al*, *J. Am. Chem. Soc.*, 1924, **46**, 1675 (*synth*)
Ofner, A., *Helv. Chim. Acta*, 1935, **18**, 951 (*synth*)
Watanabe, H. *et al*, *CA*, 1961, **55**, 16697 (*isol, deriv*)
Shannon, J.S., *Aust. J. Chem.*, 1962, **15**, 265 (*ms*)
Hardegger, E. *et al*, *Helv. Chim. Acta*, 1963, **46**, 1171 (*isol*)
Mumford, F.E. *et al*, *Phytochemistry*, 1963, **2**, 215 (*isol*)
Torii, S. *et al*, *J. Org. Chem.*, 1979, **44**, 3305 (*synth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 381.

ent-2-Hydroxy-1,15-beyeradien-3-one H-80115

2-Hydroxy-1,15-stachadien-3-one



$C_{20}H_{28}O_2$ M 300.440
Isol. from wood of *Spirostachys africana*. Prisms (hexane). Mp 132°. $[\alpha]_D$ +49° (c, 3.2 in $CHCl_3$).

Baarschers, W.H. *et al*, *J. Chem. Soc.*, 1962, 4046 (*isol, uv, ir, pmr*)

ent-3-Hydroxy-15-beyeren-2-one H-80116

3-Hydroxy-15-stachen-2-one

$C_{20}H_{30}O_2$ M 302.456
Isol. from wood of *Spirostachys africana*. Needles (hexane). Mp 129°. $[\alpha]_D$ +30° (c, 3.3 in $CHCl_3$).

Baarschers, W.H. *et al*, *J. Chem. Soc.*, 1962, 4046 (*isol, uv, ir, pmr, ord*)

2′-Hydroxy-2,3′-bipyridine H-80117

[*2,3′-Bipyridine*]-*2′(1′*H)-*one, 9CI. 3-(2-Pyridyl)-2-pyridone*

[101002-01-1]

$C_{10}H_8N_2O$ M 172.186
Yellow cryst. (CH_2Cl_2/hexane). Mp 149-150°.

Moran, D.B. *et al*, *J. Heterocycl. Chem.*, 1986, **23**, 1071 (*synth*)

2′-Hydroxy-2,4′-bipyridine H-80118

[*2,4′-Bipyridin*]-*2′(1*H)-*one, 9CI. 4-(2-Pyridyl)-2-pyridone*

$C_{10}H_8N_2O$ M 172.186

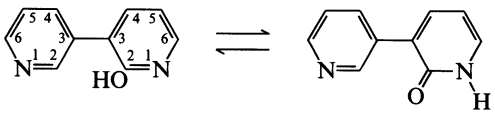
[101001-99-4]

MacBride, J.A.H. *et al*, *Tetrahedron Lett.*, 1982, **23**, 1109.
U.S. Pat., 4 450 166, (1985); *CA*, **104**, 129911t.

2-Hydroxy-3,3′-bipyridine H-80119

[*3,3′-Bipyridine*]-*2(1*H)-*one, 9CI. 3-(3-Pyridyl)-2-pyridone*

[82407-65-6]



$C_{10}H_8N_2O$ M 172.186
Pyridone tautomers prob. predominate in this series where appropriate. Off-white cryst. (2-propanol). Mp 189-192°.

MacBride, J.A.H. *et al*, *J. Chem. Res.* (*S*), 1984, **10**, 328 (*synth*)
Moran, D.B. *et al*, *J. Heterocycl. Chem.*, 1986, **23**, 1071 (*synth*)

2-Hydroxy-4,4′-bipyridine H-80120

[*4,4′-Bipyridin*]-*2(1*H)-*one, 9CI. 4-(4-Pyridyl)-2-pyridone*

$C_{10}H_8N_2O$ M 172.186

Hydrazone: [101002-00-0].
$C_{10}H_{10}N_4$ M 186.216

Yellow cryst. (CH_2Cl_2). Mp 109-110°.

U.S. Pat., 4 450 166, (1985); *CA*, **104**, 129911t (*synth*)
Moran, D.B. *et al*, *J. Heterocycl. Chem.*, 1986, **23**, 1071 (*synth*)

4-Hydroxy-2,2′-bipyridine H-80121

[*2,2′-Bipyridin*]-*4-ol*, *8CI*. *2-(2-Pyridyl)-4-pyridone*

[14712-32-4]

$C_{10}H_8N_2O$ M 172.186
Prisms (Me_2CO). Mp 145°.

Me ether: [14162-97-1]. *4-Methoxy-2,2′-bipyridine*
$C_{11}H_{10}N_2O$ M 186.213
Prisms ($CHCl_3$/hexane). Mp 67.5-68.5°.

Me ether, N-*oxide:* [14163-05-4].
$C_{11}H_{10}N_2O_2$ M 202.212
Cryst. (CH_2Cl_2/hexane). Mp 117.5-118°.

Me ether, N,N′-*dioxide:* [84175-06-4].
$C_{11}H_{10}N_2O_3$ M 218.212
Mp 242-246° dec. $Bp_{0.03}$ 180° subl.

Divekar, P.V. *et al*, *Can. J. Chem.*, 1967, **45**, 1215 (*synth*, *ir*, *uv*)
Wenkert, D. *et al*, *J. Org. Chem.*, 1983, **48**, 283 (*synth*, *ir*, *pmr*, *uv*)

4-Hydroxy-3,3′-bipyridine H-80122

[*3,3′-Bipyridin*]-*4*(*1*H)-*one*, *9CI*. *3-(3-Pyridyl)-4-pyridone*

[82407-66-7]

$C_{10}H_8N_2O$ M 172.186
Brownish plates (MeCN). Mp 222-226°. $Bp_{0.0001}$ 200° subl.

MacBride, J.A.H. *et al*, *Tetrahedron Lett.*, 1982, **23**, 1109 (*synth*, *ir*, *pmr*, *uv*)
Hull, R. *et al*, *J. Chem. Res.* (*S*), 1984, 328; *J. Chem. Res.* (*M*), 1984, 3001 (*synth*, *pmr*, *uv*)

5-Hydroxy-2,2′-bipyridine H-80123

[*2,2′-Bipyridin*]-*5-ol*, *9CI*

[1802-32-0]

$C_{10}H_8N_2O$ M 172.186
Needles ($CHCl_3$/pet. ether). Mp 157° (228-229°).

Ac: [58792-48-6].
$C_{12}H_{10}N_2O_2$ M 214.223
Cryst. (ligroin). Mp 102°.

Me ether: [58792-50-0]. *5-Methoxy-2,2′-bipyridine*, *9CI*
$C_{11}H_{10}N_2O$ M 186.213
Yellow oil which darkens in air. Mp 25°.

Otroshchenko, O.S., *CA*, 1964, **63**, 4248e (*synth*)
Kurbatov, Yu.V. *et al*, *CA*, 1966, **67**, 82059w (*synth*)
Keats, N.G. *et al*, *J. Heterocycl. Chem.*, 1976, **13**, 513 (*ms*)
Pirzada, N.H. *et al*, *Z. Naturforsch.*, *B*, 1976, **31**, 115 (*synth*, *uv*, *ir*, *pmr*,)

5-Hydroxy-2,3′-bipyridine H-80124

[*2,3′-Bipyridin*]-*5-ol*, *8CI*

[1748-06-7]

$C_{10}H_8N_2O$ M 172.186
Cryst. (MeOH). Mp 184-185° (177-179°).

Picrate: Cryst. (H_2O). Mp 217-219°.

Otroshchenko, O.S. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1954, **24**, 1661 (*synth*)
Otroshchenko, O.S. *et al*, *CA*, 1964, **63**, 3008e (*synth*)
Leont'ev, V.B. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1965, **35**, 298 (*uv*)
Leont'ev, V.B. *et al*, *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 1966, **2**, 433 (*ir*, *struct*)

5-Hydroxy-3,3′-bipyridine H-80125

[*3,3′-Bipyridin*]-*5-ol*, *8CI*

[15862-23-4]

$C_{10}H_8N_2O$ M 172.186
Mp 146-147°.

Kurbatov, Yu.V. *et al*, *CA*, 1966, **67**, 82059w (*synth*)
Otroshchenko, O.S. *et al*, *CA*, 1966, **67**, 99969r (*synth*)

6-Hydroxy-2,2′-bipyridine H-80126

[*2,2′-Bipyridin*]-*6*(*1*H)*one*, *9CI*. *6-(2-Pyridyl)-2-pyridone*

[101001-90-5]

$C_{10}H_8N_2O$ M 172.186
Off-white cryst. (CH_2Cl_2/hexane). Mp 124-127°.

Moran, D.B. *et al*, *J. Heterocycl. Chem.*, 1986, **23**, 1071 (*synth*, *pmr*)

6-Hydroxy-2,3′-bipyridine H-80127

[*2,3′-Bipyridin*]-*6*(*1*H)-*one*, *9CI*. *6-(3-Pyridyl)-2-pyridone*

[39883-44-8]

$C_{10}H_8N_2O$ M 172.186

[39883-46-0]

U.K. Pat., 1 322 318, (1973); *CA*, **79**, 105231k.

6-Hydroxy-2,4′-bipyridine H-80128

[*2,4′-Bipyridin*]-*6*(*1*H)-*one*, *9CI*. *6-(4-Pyridyl)-2-pyridone*

[39883-33-5]

$C_{10}H_8N_2O$ M 172.186

[39883-35-7]

U.K. Pat., 1 322 318, (1973); *CA*, **79**, 105231k.

6-Hydroxy-3,3′-bipyridine H-80129

[*3,3′-Bipyridin*]-*6*(*1*H)-*one*, *9CI*. *5-(3-Pyridyl)-2-pyridone*

$C_{10}H_8N_2O$ M 172.186
Hydrazone synthesised.

[101001-98-3]

U.S. Pat., 4 450 166, (1985); *CA*, **104**, 129911t (*synth*)

6-Hydroxy-3,4′-bipyridine H-80130

[*3,4′-Bipyridin*]-*6*(*1*H)-*one*. *5-(4-Pyridyl)-2-pyridone*

[62749-34-2]

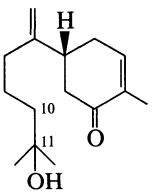
$C_{10}H_8N_2O$ M 172.186
Mp 259-260°. Several patented syntheses in addition to the ref. quoted.

Me ether: [106154-27-2]. *6-Methoxy-3,4′-bipyridine*, *9CI*
$C_{11}H_{10}N_2O$ M 186.213
Cryst. (CH_2Cl_2/hexane). Mp 60-61°.

[82718-36-3]

Fang, W.-P. *et al*, *Heterocycles*, 1986, **24**, 1585 (*synth*, *ir*, *pmr*)

11-Hydroxy-2,7(14)-bisaboladien-4-one H-80131



$C_{15}H_{24}O_2$ M 236.353
Constit. of *Mikania shushunensis*. Oil. $[\alpha]_D^{24}$ −13.2° (c, 1.8 in $CHCl_3$).

Gutierrez, A.B. *et al*, *Phytochemistry*, 1988, **27**, 3871.

10-Hydroxy-2,7(14),11-bisabolatrien-4-one H-80132

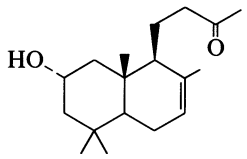
[119765-83-2]

$C_{15}H_{22}O_3$ M 250.337

Constit. of *Mikania shushunensis*. Oil. $[\alpha]_D^{25}$ −16.2° (c, 0.5 in $CHCl_3$).

Gutierrez, A.B. *et al*, *Phytochemistry*, 1988, **27**, 3871.

2-Hydroxy-14,15-bisnor-7-labden-13-one H-80133



$C_{18}H_{30}O_2$ M 278.434

2α-form

Constit. of *Waitzia acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

4-Hydroxy-2-butenoic acid, 9CI H-80134

Updated Entry replacing H-01416

4-Hydroxycrotonic acid, 8CI

$HOCH_2CH{=}CHCOOH$

$C_4H_6O_3$ M 102.090

(E)-form [24587-49-3]

Cryst. (EtOAc). Mp 107°. Readily undergoes polycondensation.

Et ester: [10080-68-9].

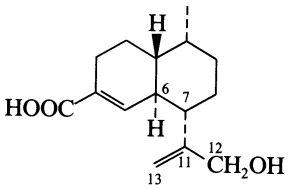
$C_6H_{10}O_3$ M 130.143

d_4^{17} 1.077. Bp_{13} 119-120°. n_D^{23} 1.461.

Laporte, J.F. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 1340 (*synth, ir, pmr*)

Takano, S. *et al*, *Synthesis*, 1974, 42 (*lactone*)

12-Hydroxy-4,11(13)-cadinadien-15-oic acid H-80135



Absolute configuration

$C_{15}H_{22}O_3$ M 250.337

Constit. of *Eremophila virgata*. New stereochemical class in the cadinane series.

11,13-Epoxy, 12-deoxy: 11,13-Epoxy-4-cadinen-15-oic acid

$C_{15}H_{22}O_3$ M 250.337

Constit. of *E. virgata*. Needles (Et_2O). Mp 180-181°. $[\alpha]_D$ +117° (c, 0.9 in $CHCl_3$).

11R,13-Dihydro: 12-Hydroxy-4-cadinen-15-oic acid

$C_{15}H_{24}O_3$ M 252.353

Constit. of *E. virgata*.

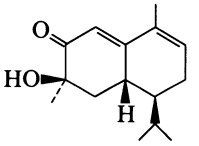
6,7-Diepimer:

$C_{15}H_{22}O_3$ M 250.337

Constit. of *E. virgata*.

Ghisalberti, E.L. *et al*, *Tetrahedron*, 1989, **45**, 6297 (*cryst struct*)

4-Hydroxy-1,9-cadinadien-3-one H-80136



$C_{15}H_{22}O_2$ M 234.338

Me ether: 4-Methoxy-1,9-cadinadien-3-one

$C_{16}H_{24}O_2$ M 248.364

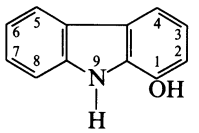
Constit. of *Senecio tomentosus*. Oil. $[\alpha]_D^{24}$ +28° (c, 0.36 in $CHCl_3$).

Mericli, A.H. *et al*, *Phytochemistry*, 1989, **28**, 1149.

1-Hydroxycarbazole H-80137

9H-Carbazol-1-ol, 9CI

[61601-54-5]



$C_{12}H_9NO$ M 183.209

Long needles (H_2O). Mp 160°.

Picrate: Orange needles (H_2O). Mp 191-192°.

Ac:

$C_{14}H_{11}NO_2$ M 225.246

Small prisms (H_2O). Mp 132-133°.

Me ether: [4544-87-0]. *1-Methoxy-9H-carbazole*

$C_{13}H_{11}NO$ M 197.236

Long needles (EtOH). Mp 69-70°.

Et ether: [115663-18-8]. *1-Ethoxy-9H-carbazole*

$C_{14}H_{13}NO$ M 211.263

Needles (pet. ether). Mp 93.5-94.5°. $Bp_{2.4}$ 185-200°.

Barnes, C.S. *et al*, *J. Chem. Soc.*, 1949, 1381 (*synth, deriv*)

Martin, T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 235 (*ethers, uv, ir, ms*)

11-Hydroxy-3,6-cholestanedione H-80138

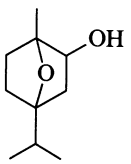
$C_{27}H_{44}O_3$ M 416.643

(5α,11α)-form

Constit. of *Acantophora spicifera*. Cryst. (MeOH). Mp 145°. $[\alpha]_D^{25}$ −11.1°.

Prakash, O. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 686 (*isol, cmr, pmr*)

2-Hydroxy-1,4-cineole H-80139



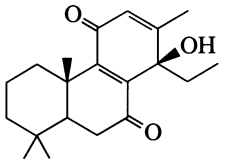
$C_{10}H_{18}O_2$ M 170.251

Constit. of *Ferula jaeschkaena*. Cryst. Mp 75°.

Garg, S.N. *et al*, *Phytochemistry*, 1989, **28**, 634.

14-Hydroxy-8,12-cleistanthadiene-7,11-dione H-80140

[119725-17-6]

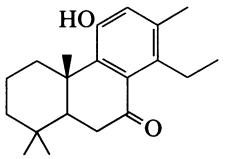


$C_{20}H_{28}O_3$ M 316.439
Constit. of *Vellozia nivea*. Yellow cryst. Mp 113-115°. $[\alpha]_D^{25}$ −4.7° (c, 0.85 in MeOH).

Pinto, A.C. *et al*, *Phytochemistry*, 1988, **27**, 3973.

11-Hydroxy-8,11,13-cleistanthatrien-7-one H-80141

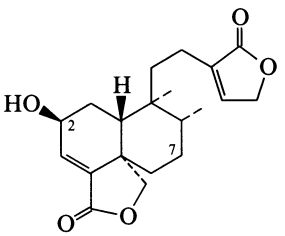
[119725-18-7]



$C_{20}H_{28}O_2$ M 300.440
Constit. of *Vellozia nivea*. Cryst. Mp 236-238°. $[\alpha]_D^{25}$ +70° (c, 0.5 in $CHCl_3$).

Pinto, A.C. *et al*, *Phytochemistry*, 1988, **27**, 3973.

ent-2α-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide H-80142



$C_{20}H_{26}O_5$ M 346.422

Ac: ent-2α-*Acetoxy*-3,13-*clerodadiene*-16,15:18,19-*diolide*
$C_{22}H_{28}O_6$ M 388.460
Constit. of *Salvia melissodora*. Cryst. (CH_2Cl_2/MeOH). Mp 202-204°. $[\alpha]_D^{20}$ −209.5° (c, 0.16 in $CHCl_3$).

7α-Hydroxy: ent-2α,7β-*Dihydroxy*-3,13-*clerodadiene*-16,15:18,19-*diolide*
$C_{20}H_{26}O_6$ M 362.422
Constit. of *S. melissodora*. Cryst. (Me_2CO/hexane). Mp 190-192°. $[\alpha]_D^{20}$ −177.6° (c, 0.2 in MeOH).

7α-Acetoxy: ent-7β-*Acetoxy*-2α-*hydroxy*-3,13-*clerodadiene*-16,15:18,19-*diolide*
$C_{22}H_{28}O_7$ M 404.459
Constit. of *S. melissodora*. Cryst. (Me_2CO/hexane). Mp 236-239°. $[\alpha]_D^{25}$ −123.9° (c, 0.184 in $CHCl_3$).

7α-Hydroxy, 2-Ac: ent-2α-*Acetoxy*-7β-*hydroxy*-3,13-*clerodadiene*-16,15:18,19-*diolide*
$C_{22}H_{28}O_7$ M 404.459
Constit. of *S. melissodora*. Cryst. (CH_2Cl_2/diisopropyl ether). Mp 197-199°. $[\alpha]_D^{20}$ −207° (c, 0.167 in $CHCl_3$).

7-Oxo: ent-2α-*Acetoxy*-7-*oxo*-3,13-*clerodadiene*-16,15:18,19-*diolide*
$C_{20}H_{24}O_6$ M 360.406
Constit. of *S. melissodora*. Cryst. (CH_2Cl_2/hexane). Mp 238-240°. $[\alpha]_D^{20}$ −239.8° (c, 0.171 in $CHCl_3$).

Esquivel, B. *et al*, *Phytochemistry*, 1989, **28**, 561.

ent-7β-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide H-80143

$C_{20}H_{26}O_5$ M 346.422
Constit. of *Salvia melissodora*. Cryst. (Me_2CO/diisopropyl ether). Mp 178-179°. $[\alpha]_D^{20}$ −154.5° (c, 0.165 in $CHCl_3$).

Ac: ent-7β-*Acetoxy*-3,13-*clerodadiene*-16,15:18,19-*diolide*
$C_{22}H_{28}O_6$ M 388.460
Constit. of *S. melissodora*. Cryst. (CH_2Cl_2/diisopropyl ether). Mp 178-179°. $[\alpha]_D^{20}$ −110.7° (c, 0.17 in $CHCl_3$).

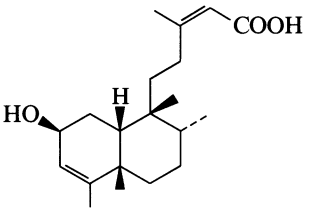
7-Epimer: ent-7α-*Hydroxy*-3,13-*clerodadiene*-16,15:18,19-*diolide*
$C_{20}H_{26}O_5$ M 346.422
Constit of *S. melissodora*. Cryst. (EtOAc/MeOH). Mp 196-197°. $[\alpha]_D^{20}$ −93.3° (c, 0.15 in MeOH).

7-Ketone: ent-7-*Oxo*-3,13-*clerodadiene*-16,15:18,19-*olide*
$C_{20}H_{24}O_5$ M 344.407
Constit. of *S. melissodora*. Cryst. (EtOAc). Mp 89-93°. $[\alpha]_D^{20}$ −168.4° (c, 0.152 in $CHCl_3$).

Esquivel, B. *et al*, *Phytochemistry*, 1989, **28**, 561.

ent-2α-Hydroxy-3,13-clerodadien-15-oic acid H-80144

[118173-04-9]



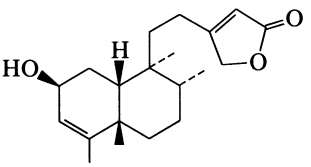
$C_{20}H_{32}O_3$ M 320.471
Constit. of *Ageratina saltillensis*.

2-Ketone: [118243-69-9]. **ent-*2-Oxo-3,13-clerodadien-15-oic acid***
$C_{20}H_{30}O_3$ M 318.455
Constit. of *A. saltillensis*.

Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187.

ent-2α-Hydroxy-3,13-clerodadien-15,16-olide H-80145

[118173-03-8]

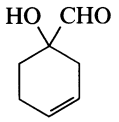


$C_{20}H_{30}O_3$ M 318.455
Constit. of *Ageratina saltillensis*.

Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 3187.

1-Hydroxy-3-cyclohexene-1-carboxaldehyde H-80146

1-Formyl-3-cyclohexenol



$C_7H_{10}O_2$ M 126.155

Ac: [55638-24-9].
$C_9H_{12}O_3$ M 168.192
Oil. $Bp_{0.1}$ 90°.

Me ether: [117370-82-8]. *1-Methoxy-3-cyclohexene-1-carboxaldehyde. 3-Formyl-3-methoxycyclohexene*
$C_8H_{12}O_2$ M 140.182
Liq.

Me ether, oxime: [117370-83-9].
$C_8H_{13}NO_2$ M 155.196
Solid. Mp 77-78°.

Hassner, A. *et al*, *J. Org. Chem.*, 1975, **40**, 3427 (*synth, pmr*)
Rubottom, G.M. *et al*, *Tetrahedron*, 1983, **39**, 861 (*synth*)
Wu, P.-L. *et al*, *J. Org. Chem.*, 1988, **53**, 5998 (*synth, pmr, ir, cmr*)

6-Hydroxydecanoic acid, 9CI H-80147

[16899-10-8]

$H_3C(CH_2)_3CH(OH)(CH_2)_4COOH$

$C_{10}H_{20}O_3$ M 188.266
Present in lipid fraction of royal jelly.

Lactone:
$C_{10}H_{18}O_2$ M 170.251
$Bp_{1.3}$ 96°. n_D^{20} 1.4601.

Netherlands Pat., 100 368, (1962); *CA*, **60**, 2783c (*synth, lactone*)
Japan. Pat., 74 85 276, (1974); *CA*, **82**, 71817a (*use*)
Lercker, G. *et al*, *Lipids*, 1981, **16**, 912 (*anal*)

7-Hydroxydecanoic acid, 9CI H-80148

[2034-55-1]

$H_3CCH_2CH_2CH(OH)(CH_2)_5COOH$

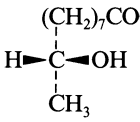
$C_{10}H_{20}O_3$ M 188.266
Present in hydrolysate of leaf resin of *Ipomoea fistulosa* and saponified cells of *Mucor* spp. Liq.

[73276-73-0]

Legler, G., *Phytochemistry*, 1965, **4**, 29 (*isol*)
Satoshi, T. *et al*, *Agric. Biol. Chem.*, 1980, **44**, 193 (*synth, ms, isol, ir, glc*)

9-Hydroxydecanoic acid, 9CI H-80149

[1422-27-1]



(R)-form

$C_{10}H_{20}O_3$ M 188.266
Present in *Agaricus campestris*, *Mucor hiemalis* and royal jelly.

(R)-form [35433-73-9]
Oil. Mp 32°. $[\alpha]_D$ −7.5° (MeOH), $[\alpha]_D^{23}$ −8.1° (c, 0.11 in $CHCl_3$).

Me ester:
$C_{11}H_{22}O_3$ M 202.293
$Bp_{0.005}$ 78-80°. $[\alpha]_D$ −9.5° (c, 1.45 in cyclohexane).

tert-*Butyl ester:*
$C_{14}H_{28}O_3$ M 244.373
$[\alpha]_D$ −7.0° (c, 1.73 in cyclohexane).

Lactone: [74183-94-1]. *10-Methyl-2-oxecanone, 9CI.* ***Phoracantholide I***
$C_{10}H_{18}O_2$ M 170.251
Present in metasternal gland of *Phoracantha synonyma*.
$[\alpha]_D^{22}$ −37.4° (c, 0.02 in $CHCl_3$).

(S)-form [35433-72-8]
$[\alpha]_D^{22}$ +8.14° (c, 0.14 in $CHCl_3$).

Me ester: Oil. $Bp_{0.002}$ 80°. $[\alpha]_D$ +9.3° (c, 2.0 in cyclohexane).

Lactone: $[\alpha]_D^{22}$ +38.38° (c, 0.16 in $CHCl_3$).

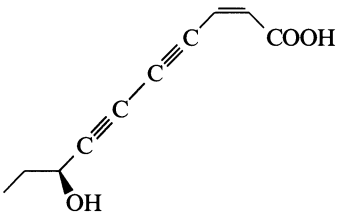
(±)-form [40151-97-1]

Me ester: $Bp_{0.01}$ 85°.

tert-*Butyl ester:* $Bp_{0.01}$ 72-74°.

Moore, B.P. *et al*, *Aust. J. Chem.*, 1976, **29**, 1365 (*isol*)
Gerlach, H. *et al*, *Helv. Chim. Acta*, 1978, **61**, 1226 (*synth, ir, pmr, ms*)
Fink, M. *et al*, *Helv. Chim. Acta*, 1982, **65**, 2563 (*derivs*)
Tressl, R. *et al*, *J. Agric. Food Chem.*, 1982, **30**, 89 (*glc, ms*)
Voss, G. *et al*, *Helv. Chim. Acta*, 1983, **66**, 2294 (*synth*)
Clarke, M.J. *et al*, *J. Liq. Chromatogr.*, 1986, **9**, 1711 (*hplc*)
Naoshima, Y. *et al*, *Chem. Lett.*, 1987, 2379 (*synth, lactone*)

8-Hydroxy-2-decene-4,6-diynoic acid, 9CI H-80150



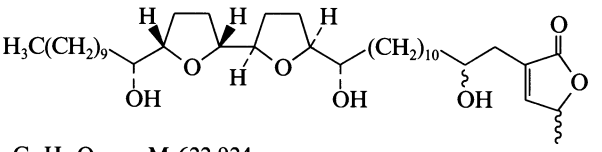
$C_{10}H_{10}O_3$ M 178.187

(S,E)-form [56085-68-8]
Isol. from *Aster novi belgii*. Needles (Et_2O/pet. ether). Mp 97-100°.

O-*Angeloyl, Me ester:* [24486-36-0]. ***8-Angeloyloxylachnophyllum ester***
$C_{16}H_{18}O_4$ M 274.316
Liq. $Bp_{0.001}$ 120-130° part dec. . $[\alpha]_D^{20}$ −164° (c, 0.85 in Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 3469; 1965, **98**, 2608 (*isol, uv, ir, pmr, ms, abs config*)
Ord, M.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 687 (*synth, uv, ir, pmr*)

4-Hydroxy-25-desoxyneorollinicin H-80151

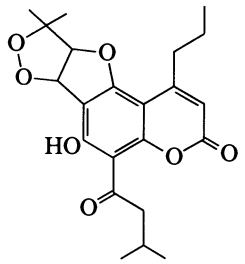


$C_{37}H_{66}O_7$ M 622.924
Constit. of *Rollinia papilionella*. Wax. Mp 25°.

Abreo, M.J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 822 (*isol, pmr, cmr*)

6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3*H*,9*H*-[1,2]-dioxolo-[3′,4′:4,5]furo[2,3-*f*][1]benzopyran-3-one, 9CI **H-80152**

[30390-08-0]



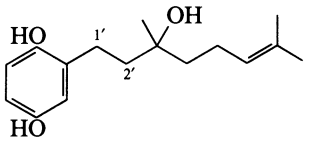
$C_{22}H_{26}O_7$ M 402.443

Isol. from *Mammea americana*. An oxidn. prod. of Mammein. Mp 181-182°. The isomer having a 2-methylbutanoyl side-chain cooccurs.

[30390-09-1]

Crombie, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 2241.
Finnegan, R.A. *et al*, *J. Pharm. Sci.*, 1972, **61**, 1603 (*isol, ir, uv, pmr*)

2-(3-Hydroxy-3,7-dimethyl-6-octenyl)-1,4-benzenediol **H-80153**



$C_{16}H_{24}O_3$ M 264.364

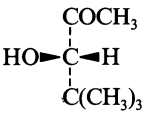
Metab. of *Amaroucium multiplicatum*. Oil.

1′,2′-Didehydro (E-)*: 2-(3-Hydroxy-3,7-dimethyl-2,6-octadienyl)-1,4-benzenediol*
$C_{16}H_{22}O_3$ M 262.348
Metab. of *A. multiplicatum*. Oil.

Sato, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 975 (*isol, pmr, cmr*)

3-Hydroxy-4,4-dimethyl-2-pentanone, 9CI **H-80154**

*Acetyl-*tert*-butylcarbinol*



(*S*)-*form*

$C_7H_{14}O_2$ M 130.186

(*S*)-*form* [97869-13-1]
Oil. Bp_1 45-50°. $[\alpha]_D^{25}$ +133.2° (c, 1 in $CHCl_3$).

(±)-*form*
d_4^{25} 0.92. $Bp_{0.35}$ 26°.

Semicarbazone: Cryst. (EtOH aq.). Mp 192-193°.

Stacy, G.W. *et al*, *J. Org. Chem.*, 1966, **31**, 1753.
Zhang, W.-Y. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4652 (*synth, ir, pmr, cmr*)

5-Hydroxy-5,5-diphenylpentanoic acid **H-80155**

[68719-02-8]

$Ph_2C(OH)CH_2CH_2CH_2COOH$

$C_{17}H_{18}O_3$ M 270.327
Cryst. Mp 132-134°.

Lehmann, J. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 827 (*synth, pmr*)

7-Hydroxydodecanoic acid, 9CI **H-80156**

[70393-62-3]

$H_3C(CH_2)_4CH(OH)(CH_2)_5COOH$

$C_{12}H_{24}O_3$ M 216.320

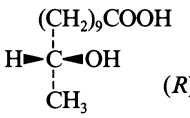
(±)-*form* [73276-74-1]
Mp 55.5-56.5°. (*R*)-form also known.

[58262-37-6, 78737-61-8]

Tahera, S. *et al*, *Agric. Biol. Chem.*, 1980, **44**, 193 (*synth, ir, ms, glc*)
Midland, M.M. *et al*, *J. Org. Chem.*, 1981, **46**, 3933 (*synth, pmr*)

11-Hydroxydodecanoic acid, 9CI **H-80157**

[32459-66-8]



(*R*)-*form*

$C_{12}H_{24}O_3$ M 216.320

Constit. of royal jelly. Metab. of *Fusarium oxysporum*.

(*R*)-*form*

Me ester: [88785-25-5].
Oil. $Bp_{0.002}$ ~100°. $[\alpha]_D$ −7.7° (c, 2.15 in cyclohexane).

(±)-*form* [83515-89-3]
Cryst. (Et_2O/pet. ether). Mp 54°.

Me ester: [109718-22-1].
$C_{13}H_{26}O_3$ M 230.347
Liq. or cryst. Bp_7 160°.

Anilide: Small prisms (pet. ether). Mp 87°.

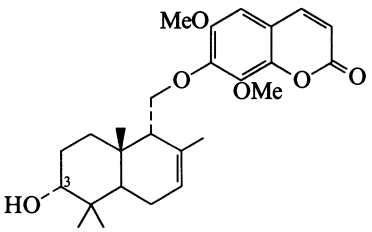
Lactone: 11-Decanolide. Dihydrorecifeiolide
$C_{12}H_{22}O_2$ M 198.305
Oil. $Bp_{0.001}$ 65-70°.

[66605-95-6]

Ellin, A. *et al*, *Arch. Biochem. Biophys.*, 1973, **158**, 597 (*synth, derivs*)
Voss, G. *et al*, *Helv. Chim. Acta*, 1983, **66**, 2294 (*synth, ir, pmr, cmr*)
Hesse, B. *et al*, *Helv. Chim. Acta*, 1984, **67**, 1713; 1986, **69**, 1323 (*lactone*)
Makita, A. *et al*, *J. Antibiot.*, 1986, **39**, 1257 (*synth, derivs*)

7-*O*-(3-Hydroxy-7-drimen-11-yl) isofraxidin **H-80158**

[52418-68-5]



$C_{26}H_{34}O_6$ M 442.551

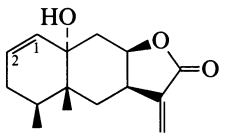
Isol. from *Artemisia pontica*. Mp 129.5°. $[\alpha]_D^{23}$ +201° (Me_2CO).

3-Ketone: [57194-40-8].
$C_{26}H_{32}O_6$ M 440.535
Isol. from *Anthemis aciphylla*. Mp 130°. $[\alpha]_D^{22}$ +156.3° ($CHCl_3$).

[52329-14-3, 52329-15-4]

Bohlmann, F. *et al*, *Chem. Ber.*, 1974, **107**, 644; 1975, **108**, 1902.

10-Hydroxy-1,11(13)-eremophiladien-12,8-olide H-80159



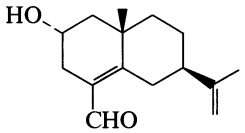
$C_{15}H_{20}O_3$ M 248.321

(8β,10α)-form
Constit. of *Ondetia linearis*. Oil.

1α,2α-Epoxide: 1α,2α-Epoxy-10α-hydroxy-11(13)-eremophilen-12,8β-olide
$C_{15}H_{20}O_4$ M 264.321
Constit. of *O. linearis*. Oil.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

2-Hydroxy-4,11(13)-eudesmadien-15-al H-80160

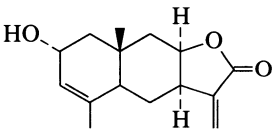


$C_{15}H_{22}O_2$ M 234.338

2α-form [119863-97-7]
$C_{15}H_{22}O_2$ M 234.338
Constit. of *Tetragonotheca ludoviciana*. Oil. $[\alpha]_D^{24}$ +51° (c, 0.7 in $CHCl_3$).

Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3881.

2-Hydroxy-3,11(13)-eudesmadien-12,8-olide H-80161



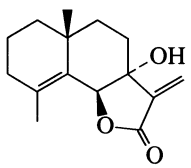
$C_{15}H_{20}O_3$ M 248.321

(2α,8β)-form
Constit. of *Ondetia linearis*.

Ac: Cryst. Mp 153°. $[\alpha]_D^{24}$ +71° (c, 0.27 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

7-Hydroxy-4,11(13)-eudesmadien-12,6-olide H-80162

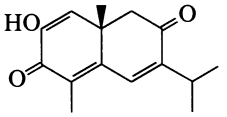


$C_{15}H_{20}O_3$ M 248.321

(6β,7α)-form
7-Hydroxyfrullanolide
Constit. of *Sphaeranthus indicus*. Shows antimicrobial props. Cryst. (pet. ether). Mp 59-60°. $[\alpha]_D^{24}$ −39° (c, 4.0 in MeOH).

Atta-ur-Rahman, *J. Chem. Res.* (*S*), 1989, 68.

2-Hydroxy-1,4,6-eudesmatriene-3,8-dione H-80163

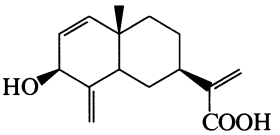


$C_{15}H_{18}O_3$ M 246.305
Constit. of *Baccharis boliviensis*. Cryst. Mp 96°. $[\alpha]_D^{24}$ +123° (c, 0.49 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

3-Hydroxy-1,4(15),11(13)-eudesmatrien-12-oic acid H-80164

3-Hydroxy-1,2-dehydrocostic acid



$C_{15}H_{20}O_3$ M 248.321

3β-form
Me ester:
$C_{16}H_{22}O_3$ M 262.348
Constit. of *Centaurea arguta*. Oil.

3-Ketone, Me ester: Methyl 3-oxo-1,4(15),11(13)-eudesmatrien-12-oate
$C_{16}H_{20}O_3$ M 260.332
Constit. of *C. arguta*. Oil.

Gadeschi, E. *et al*, *Phytochemistry*, 1989, **28**, 2204 (*isol*, *pmr*)

2-Hydroxy-5-eudesmen-12,8-olide H-80165

$C_{15}H_{22}O_3$ M 250.337

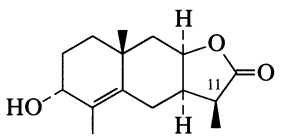
(2α,8β,11αH)-form
2α-Hydroxy-11α,13-dihydroalantolactone
Constit. of *Ondetia linearis*. Cryst. Mp 147°.

11α-Hydroxy: 2α,11α-Dihydroxy-5-eudesmen-12,8β-olide.
2α,11α-Dihydroxy-11,13-dihydroalantolactone
$C_{15}H_{22}O_4$ M 266.336
Constit. of *O. linearis*. Cryst. Mp 186°. $[\alpha]_D^{24}$ −26° (c, 0.16 in $CHCl_3$).

(2α,8β,11βH)-form
2α-Hydroxy-11β,13-dihydroalantolactone
Constit. of *O. linearis*. Cryst. Mp 134°. $[\alpha]_D^{24}$ +9° (c, 0.18 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

3-Hydroxy-4-eudesmen-12,8-olide H-80166



(3α,8β,11α*H*)-*form*

$C_{15}H_{22}O_3$ M 250.337

(3α,8β,11αH)-form

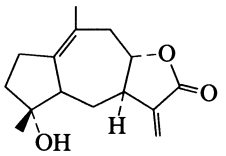
Constit. of *Ondetia linearis*. Cryst. Mp 123°. $[\alpha]_D^{24}$ +99° (c, 0.54 in $CHCl_3$).

(3β,8β,11βH)-form

Constit. of *O. linearis*. Gum. $[\alpha]_D^{24}$ +145° (c, 0.12 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

4-Hydroxy-1(10),11(13)-guaiadien-12,8-olide H-80167

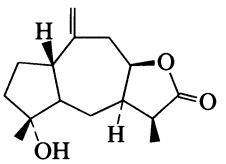


$C_{15}H_{20}O_3$ M 248.321

Constit. of *Helichrysum dasyanthum*. Gum.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

4-Hydroxy-10(14)-guaien-12,8-olide H-80168

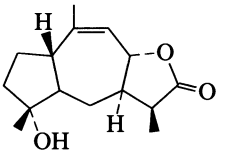


$C_{15}H_{22}O_3$ M 250.337

Constit. of *Helichrysum splendidum*. Gum.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

4-Hydroxy-9-guaien-12,8-olide H-80169



$C_{15}H_{22}O_3$ M 250.337

Constit. of *Helichrysum splendidum*. Cryst. Mp 113°. $[\alpha]_D^{24}$ −99° (c, 0.19 in $CHCl_3$).

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

10-Hydroxy-16-hentriacontanone H-80170

10-Hydroxypalmitone

[87264-34-4]

$$H_3C(CH_2)_8CH(OH)(CH_2)_5CO(CH_2)_{14}CH_3$$

$C_{31}H_{62}O_2$ M 466.830

Isol. from leaf wax of *Santalum album* and from *Machilus glaucescens*. Plates (Me_2CO). Mp 96-97°.

Ac: Mp 39.5-40.0°.

Oxime: Mp 63.4-63.6°.

Chibnall, A.C. *et al*, *Biochem. J.*, 1937, **31**, 1981 (*isol, struct, synth*)
Talapatra, B. *et al*, *J. Indian Chem. Soc.*, 1982, **59**, 1364 (*isol*)

8-Hydroxy-5-hentriacontanone H-80171

$$H_3C(CH_2)_{22}CH(OH)CH_2CH_2CO(CH_2)_3CH_3$$

$C_{31}H_{62}O_2$ M 466.830

Constit. of roots of *Costus speciosus*. Cryst. (MeOH). Mp 84-85°.

Gupta, M.M. *et al*, *Phytochemistry*, 1981, **20**, 2553.

11-Hydroxyhexadecanoic acid H-80172

Updated Entry replacing H-01877

11-Hydroxypalmitic acid. Jalapinolic acid. Scammonolic acid

$$H_3C(CH_2)_4CH(OH)(CH_2)_9COOH$$

$C_{16}H_{32}O_3$ M 272.427

(+)-form [502-75-0]

Occurs in jalap and Scammony resins (*Ipomoea orizabensis* and *Convolvulus scammonia*) and other *I.* spp., in glycosidic form. Cryst. (EtOAc). Mp 68-69°. $[\alpha]_D$ +0.79° ($CHCl_3$).

Me ester: [60368-18-5].

$C_{17}H_{34}O_3$ M 286.454

Cryst. (pet. ether or EtOAc). Mp 40.5-41.5°, Mp 47-49°. Bp_3 183-186°.

Et ester:

$C_{18}H_{36}O_3$ M 300.481

Cryst. Mp 47-48°.

Ac:

$C_{18}H_{34}O_4$ M 314.464

Oil. Bp_{50} 224-225°.

O-[*α-L-Rhamnopyranosyl(1→4)-α-L-rhamnopyranoside*]: [68124-11-8]. ***Muricatin B***

$C_{28}H_{52}O_{11}$ M 564.712

Isol. from *I. muricata*. Syrup. $[\alpha]_D^{26}$ −56.6° (c, 0.495 in EtOH)(synthetic).

O-Glycoside: Jalapinic acid. Scammoninic acid. Scammonic acid

Isol. from *I. orizabensis* and *C. scammonia*. Hygroscopic solid. Mp 66°. Gives Jalapinolic acid, glucose, rhamnose and rhodeose on hydrol. May not be homogeneous.

(±)-form

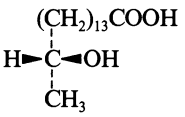
Cryst. (EtOAc). Mp 68-69°.

Me ester: Cryst. (pet. ether). Mp 40.5-41.5°. Bp_3 183-186°.

Power, F.B. *et al*, *J. Chem. Soc.*, 1912, **101**, 398 (*isol*)
Davies, C.A. *et al*, *J. Am. Chem. Soc.*, 1928, **50**, 1754 (*synth*)
Bauer, K.H. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1934, **272**, 841 (*Jalapinic acid*)
Smith, C.R. *et al*, *Phytochemistry*, 1964, **3**, 289 (*isol*)
Khanna, S.N. *et al*, *Phytochemistry*, 1967, **6**, 735.
Tulloch, A.P., *Phytochemistry*, 1976, **15**, 1153 (*isol*)
Wagner, H. *et al*, *Phytochemistry*, 1977, **16**, 715 (*glc, ms*)
Liptak, A. *et al*, *Phytochemistry*, 1978, **17**, 997 (*Muricatin B*)

15-Hydroxyhexadecanoic acid H-80173

Updated Entry replacing H-00541



(R)-form

$C_{16}H_{32}O_3$ M 272.427

(R)-form

Lactone: [69297-56-9]. *15-Hexadecanolide. 16-Methyloxacyclohexadecan-2-one, 9CI*

$C_{16}H_{30}O_2$ M 254.412

Constit. of Galbanum absolute (from *Ferula galbaniflua* and *F. rubicaulis*). $[\alpha]_D^{20}$ −16.5° (c, 1.03 in $CHCl_3$).

(S)-form

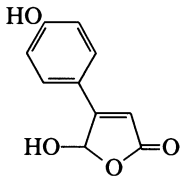
Lactone: Oil. $Bp_{0.05}$ 110-115°. $[\alpha]_D^{20}$ +2.41° (c, 1.66 in $CHCl_3$).

(±)-form

Lactone: $Bp_{0.06}$ 130°.

Becker, J. *et al*, *Helv. Chim. Acta*, 1971, **54**, 2889 (*synth*)
Kaiser, R. *et al*, *Helv. Chim. Acta*, 1978, **61**, 2671 (*isol, synth*)
Kostova, K. *et al*, *Helv. Chim. Acta*, 1984, **67**, 1713 (*synth, pmr, cmr*)
Stanchev, S. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1052 (*synth, abs config, bibl*)

5-Hydroxy-4-(4-hydroxyphenyl)-2(5*H*)-furanone H-80174

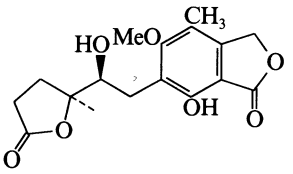


$C_{10}H_8O_4$ M 192.171
Constit.of *Sphagnum* spp. Needles (H_2O). Mp 228°. $[\alpha]_D^{20}$ −3.5° (c, 0.55 in MeOH).

Wilschke, J. *et al*, *Phytochemistry*, 1989, **28**, 1725.

7-Hydroxy-6-[2-hydroxy-2-(tetrahydro-2-methyl-5-oxo-2-furyl)ethyl]-5-methoxy-4-methylphthalide,8CI H-80175

7-Hydroxy-6-[2-hydroxy-2-(2-methyl-5-oxotetrahydro-2-furyl)ethyl]-5-methoxy-4-methyl-1-phthalanone



Relative configuration

$C_{17}H_{20}O_7$ M 336.341
Prob. rel. config. shown (descr. as *'threo'*). Isol. from *Penicillium brevi-compactum* cultures. Cryst. (Me_2CO/pet. ether). Mp 218-220°.

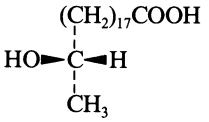
[26644-06-4]

Campbell, I.M. *et al*, *Tetrahedron Lett.*, 1966, 5107 (*isol, uv, ir, pmr, ms, struct*)
Jones, D.F. *et al*, *J. Chem. Soc. C*, 1970, 1725 (*isol, pmr*)

19-Hydroxyicosanoic acid H-80176

19-Hydroxyeicosanoic acid, 9CI. 19-Hydroxyarachidic acid

[34383-23-8]



$C_{20}H_{40}O_3$ M 328.534

(S)-form [34370-60-0]

Isol. from oil of *Torulopsis magnoliae*. Cryst. (Me_2CO). Mp 86.5-87.5°. $[\alpha]_D^{25}$ +5.2° (c, 1.4 in AcOH).

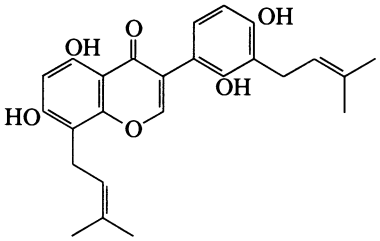
Me ester:
$C_{21}H_{42}O_3$ M 342.561
Cryst. (pet. ether). Mp 58-60°. $[\alpha]_D^{25}$ +3.6° (c, 2.4 in MeOH).

Tulloch, A.P. *et al*, *Can. J. Chem.*, 1962, **40**, 1362.

2′-Hydroxyisolupalbigenin H-80177

2′,4′,5,7-Tetrahydroxy-3′,8-diprenylisoflavone

[121747-94-2]



$C_{25}H_{26}O_6$ M 422.477
Constit. of *Lupinus albus*. Gum.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

6-Hydroxyisoquinoline H-80178

6-Isquinolinol

[7651-82-3]

C_9H_7NO M 145.160
Cryst. (2-propanol). Mp 220°.

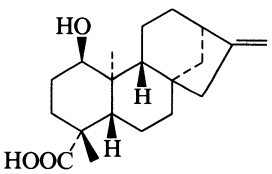
Me ether: [52986-70-6]. *6-Methoxyisoquinoline*
$C_{10}H_9NO$ M 159.187
Noncryst. or low-melting cryst. Mp 36°.

Me ether, picrate: Mp 225°.

Me ether, N-*oxide:*
$C_{10}H_9NO_2$ M 175.187
Cryst. (as hydrochloride). Mp 197° (hydrochloride).

Robinson, R.A., *J. Am. Chem. Soc.*, 1947, **69**, 1939, 1944 (*synth, deriv*)
Mason, S.F., *J. Chem. Soc.*, 1957, 4874, 5010 (*ir, uv, props, tautom*)
Hendrickson, J.B. *et al*, *J. Org. Chem.*, 1983, **48**, 3344 (*synth, deriv*)
Peet, N.P. *et al*, *J. Heterocycl. Chem.*, 1987, **24**, 715 (*ms, deriv*)

ent-1α-Hydroxy-16-kauren-19-oic acid H-80179



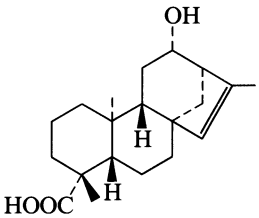
$C_{20}H_{30}O_3$ M 318.455

Ac: [122585-74-4]. ent-1α-*Acetoxy*-16-*kauren*-19-*oic acid*
$C_{22}H_{32}O_4$ M 360.492
Constit. of *Helichrysum chionosphaerum*. Gum.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

ent-12β-Hydroxy-15-kauren-19-oic acid H-80180

ent-*12β-Hydroxyisokauren-19-oic acid*



$C_{20}H_{30}O_3$ M 318.455
Constit. of *Helichrysum davenportii*. Gum. $[\alpha]_D^{24}$ −62° (c, 1.03 in $CHCl_3$).

Jacupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 543.

ent-3β-Hydroxy-16-kauren-18-oic acid H-80181

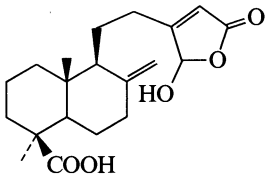
$C_{20}H_{30}O_3$ M 318.455

Ac: ent-3*β-Acetoxy*-16-*kauren*-18-*oic acid*. 3-*Acetoxykaurenic acid*
$C_{22}H_{32}O_4$ M 360.492
Constit. of *Trachylobium verrucosum*.

Ac, Me ester: Mp 130-135°. $[\alpha]_D$ −70° (c, 1.5 in $CHCl_3$).

Hugel, G. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1974; 1965, 2882, 2888 (*isol, ir, pmr, ms, struct*)

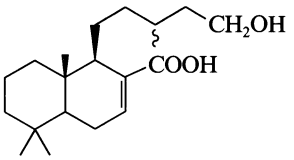
16-Hydroxy-8(17),13-labdadien-15,16-olid-19-oic acid H-80182



$C_{20}H_{28}O_5$ M 348.438
Constit. of *Calocedrus formosana*. Cryst. Mp 175-176°.

Fang, J.-M. *et al*, *Phytochemistry*, 1989, **28**, 1173.

15-Hydroxy-7-labden-17-oic acid H-80183



$C_{20}H_{34}O_3$ M 322.487
Constit. of *Halimium verticillatum*.

Me ether, Me ester: Oil. $[\alpha]_D^{22}$ −21.8° (c, 0.67 in $CHCl_3$).

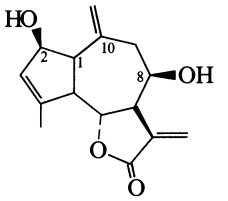
Ac:
$C_{22}H_{36}O_4$ M 364.524
Constit of *H. verticillatum*.

O-Z-*Cinnamoyl: 15Z-Cinnamoyloxy-7-labden-17-oic acid*
$C_{29}H_{42}O_4$ M 454.648
Constit. of *H. verticillatum*.

O-Z-*Cinnamoyl, Me ester:* Oil. $[\alpha]_D^{22}$ −25.5° (c, 2.1 in $CHCl_3$).

Urones, J.G. *et al*, *Phytochemistry*, 1989, **28**, 557.

2-Hydroxyligustrin H-80184



$C_{15}H_{18}O_4$ M 262.305

2β-form

8-O-(*2-methyl-2,3-epoxybutanoyl*):
$C_{20}H_{24}O_6$ M 360.406
Constit. of *Trichogonia santosii*. Oil. $[\alpha]_D^{24}$ −31° (c, 0.52 in $CHCl_3$). Diastereoisomeric epoxide also isolated.

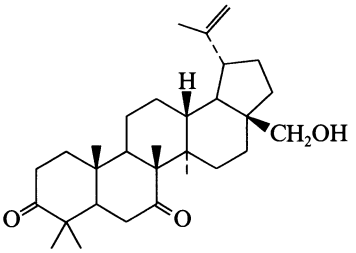
2-Ketone, 8-O-(2-methyl-2,3-epoxybutanoyl):
$C_{20}H_{22}O_6$ M 358.390
Constit. of *T. santosii*. Oil. $[\alpha]_D^{24}$ +41° (c, 0.65 in $CHCl_3$).

$\Delta^{1(10)}$-*Isomer, 2-ketone, 8*-O-(*2-methyl-2,3-epoxybutanoyl*):
8β-(2-methyl-2,3-epoxybutyroyloxy)-dehydroleucodin
$C_{20}H_{22}O_6$ M 358.390
Constit. of *T.santosii*. Oil. $[\alpha]_D^{24}$ −96° (c, 0.69 in $CHCl_3$).

Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1984, 162.

28-Hydroxy-20(29)-lupene-3,7-dione H-80185

Kanerodione



$C_{30}H_{46}O_3$ M 454.692
Constit. of *Nerium oleander*. Cryst. (EtOAc/C_6H_6). Mp 178-180°. $[\alpha]_D^{24}$ −36.36° (c, 0.11 in $CHCl_3$).

Siddiqui, S. *et al*, *Phytochemistry*, 1989, **28**, 1187.

3-Hydroxy-20(29)-lupen-11-one H-80186

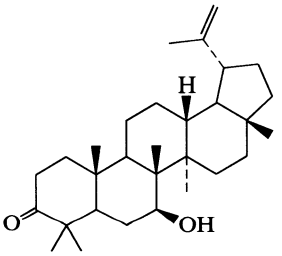
$C_{30}H_{48}O_2$ M 440.708

3α-form

11-*Oxoepilupeol*
Isol. from leaves and twigs of *Fluorensia resinosa*. Cryst. Mp 208°. $[\alpha]_D^{25}$ +34.7°.

Estrada, H. *et al*, *CA*, 1966, **64**, 3617.

7-Hydroxy-20(29)-lupen-3-one H-80187



$C_{30}H_{48}O_2$ M 440.708

7β-form

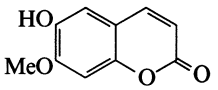
Constit. of *Salvia pratensis*. Cryst. (MeOH). Mp 217-219°. $[\alpha]_D$ +10.9° (c, 0.8 in MeOH).

Anaya, J. *et al*, *Phytochemistry*, 1989, **28**, 2206 (*isol*, *pmr*, *cmr*)

6-Hydroxy-7-methoxy-2*H*-1-benzopyran-2-one H-80188

6-Hydroxy-7-methoxycoumarin. ***Isoscopoletin***

[776-86-3]



$C_{10}H_8O_4$ M 192.171

Isol. from *Bupleurum frutescens* and *Artemisia messerschmidiana*. Yellow cryst. (H_2O). Mp 185°.

O-*β-D-Glucoside:* [20186-29-2]. ***Magnolioside***

$C_{16}H_{18}O_9$ M 354.313

Isol. from *Magnolia macrophylla*. Mp 227°. $[\alpha]_D$ −28° (Py).

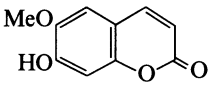
Head, F.S.H. *et al*, *J. Chem. Soc.*, 1930, 2434 (*isol*)
Plouvier, V., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. D*, 1968, **266**, 1526 (*Magnolioside*)
González, A.G. *et al*, *An. Quim.*, 1975, **71**, 109 (*isol*)

7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, 9CI H-80189

Updated Entry replacing H-70153

7-Hydroxy-6-methoxycoumarin. ***Scopoletin***. *Aesculetin 6-methyl ether. Chrysatropic acid. Gelseminic acid. β-Methylaesculetin*

[92-61-5]



$C_{10}H_8O_4$ M 192.171

Occurs widely in the plant world, for example, the root of *Gelsemium sempervirens*, *Atropa belladonna*, *Convolvulus scammonia*, *Ipomaea orizabensis*, *Prunus serotina*, *Fabiana imbricata* and also *Diospyros* spp., *Peucedanum* spp., *Heracleum* spp., *Skimmea* spp. Also occurs in the Chinese crude drug Toki(from *Angelica acutiloba*). Needles or prisms (EtOH). Mp 204°. Reduces Fehling's and Tollen's reagents.

▷ GN6930000.

Ac: Mp 177°.

O-*β-D-Glucopyranosyl:* [531-44-2]. ***Scopolin***. *Murrayin*

$C_{16}H_{18}O_9$ M 354.313

Isol. from *Scopolia japonica*, *Hedera helix* and others. Mp 217-219°.

O-(6O-*β-D-Xylopyranosyl-β-D-glucopyranoside*): [18309-73-4]. ***Fabiatrin***

$C_{16}H_{18}O_9$ M 354.313

Isol. from leaves of *Fabiana imbricata*. Needles + $2H_2O$ (H_2O). Mp 226-228°.

O-(*3-Methyl-2-butenyl*): [13544-37-1]. *6-Methoxy-7-[(3-methyl-2-butenyl)oxy]coumorin, 8CI*

$C_{15}H_{16}O_4$ M 260.289

Isol. from *Ptaeroxylon obliquum*. Mp 81-82°.

O-(*2,3-Dihydroxy-3-methylbutoxy*): [75082-72-3]. ***Obtusinin***. *7-(2′,3′-Dihydroxy-3′-methylbutyloxy)-6-methoxy-2H-1-benzopyran-2-one*

$C_{15}H_{18}O_6$ M 294.304

Isol. from *Haplophyllum obtusifolium*. Mp 136-138°.

O-(*3,7-Dimethyl-2,6-octadienyl*): [28587-43-1]. ***7-Geranyloxy-6-methoxycoumarin***

$C_{20}H_{24}O_4$ M 328.407

Isol. from *Thapsia gargonica*. Mp 84-84.5°.

Seka, R. *et al*, *Ber.*, 1931, **64**, 909.
Head, F.G.H. *et al*, *J. Chem. Soc.*, 1931, 1241 (*synth*)
McCabe, P.H. *et al*, *J. Chem. Soc. C*, 1967, 145 (*3-Methyl-2-butenyl*)
Larsen, P.K. *et al*, *Acta Chem. Scand.*, 1970, **24**, 1113 (*2,7-Dimethyl-2,6-octadienyl*)
Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985, nos. 1328, 1329 (*occur*)
Gonzalez, A.G. *et al*, *An. Quim.*, 1973, **69**, 1013 (*pmr*)
Tanaka, S. *et al*, *Arzneim.-Forsch.*, 1977, **27**, 2039 (*isol*)
Herath, W.H.M. *et al*, *Phytochemistry*, 1978, **17**, 1007 (*isol*)
Ishibura, N. *et al*, *Z. Naturforsch.*, *C*, 1979, **34**, 628.
Ahluwalia, V.K. *et al*, *Monatsh. Chem.*, 1982, **113**, 197 (*Obtusinin*)
Abu-Eittah, R.H. *et al*, *Can. J. Chem.*, 1985, **63**, 1173 (*uv*)
Koul, S.K. *et al*, *Indian J. Chem.*, *Sect. B*, 1987, **26**, 574 (*synth*)

7-Hydroxy-4′-methoxyisoflavone H-80190

Updated Entry replacing H-02182

*7-Hydroxy-3-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*. ***Formononetin***. *Formoononetin. Biochanin B. Neochanin. Pratol*

[485-72-3]

$C_{16}H_{12}O_4$ M 268.268

Constit. of red and subterranean clovers (*Trifolium pratense* and *T. subterraneum*) and of Chana (*Cicer arietinum*). Constit. of the heartwood of *Pterocarpus indicanus*. Found also in *Baptisia australis*. Widely distributed in the Leguminosae (Papilionoideae). Also in *Virola caducifolia* and *V. multinerva* (Myricaceae). Cryst. Mp 265-266° (257°).

▷ Exp. carcinogen.

Ac: Mp 171-172°.

7-O-*β-D-Glucoside:* [486-62-4]. ***Ononin***

$C_{22}H_{22}O_9$ M 430.410

Widely distributed in the Leguminosae subfamily Papilionoideae, eg. in *Amorpha fruticosa*, *Baptisia* spp., *Cicer arietinum*, *Cladrastis* spp., *Dalbergia paniculata*, *Genista patula*, *Medicago sativa*, *Ononis* spp., *Piptanthus* spp. *Pueraria thunbergiana*, *Spartium junceum*, *Thermopsis* spp., *Trifolium* spp. and *Wisteria floribunda*. Needles (dioxan aq.). Mp 218-219°.

7-O-*Laminarabioside:* [56222-47-0].

$C_{28}H_{32}O_{14}$ M 592.552

Isol. from *Cladrastis platycarpa* and *C. shikokiana*. Needles. Mp 175-176°.

7-O-*Rhammosylglucoside:*

$C_{28}H_{32}O_{13}$ M 576.553

Isol. from *B.* spp.

7-O-*Rutinoside:*

$C_{28}H_{32}O_{13}$ M 576.553

Isol. from bark of *D. paniculata*. Cryst. (C_6H_6/pet. ether) (as acetate). Mp 120-122° (acetate).

7-O-(6-O-*Malonylglucoside*): [34232-16-1].

$C_{25}H_{24}O_{12}$ M 516.457

Isol. from leaves of *Trifolium pratense* and *T. subterraneum*. Needles $+\frac{1}{2}$ H_2O (MeOH).

7-O-(6-O-*Malonylglucoside*), *Me ester:* [34232-18-3].

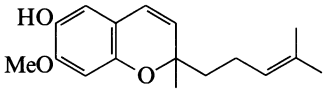
$C_{26}H_{26}O_{12}$ M 530.484

Isol. from leaves of *T. pratense* and *T. subterraneum*. Needles (MeOH). Mp 198°.

Bradbury, R.B., *J. Chem. Soc.*, 1951, 3447 (*isol*)

Bose, J.L., *J. Sci. Ind. Res., Sect. B*, 1951, **10**, 291 (*isol, struct*)
Baker, W. *et al*, *J. Chem. Soc.*, 1953, 1852 (*synth*)
Cooke, R.G., *Aust. J. Chem.*, 1964, **17**, 379 (*isol, struct*)
Lebreton, P. *et al*, *Phytochemistry*, 1967, **6**, 1675 (*isol*)
Benn, M.H., *Can. J. Chem.*, 1970, **48**, 1624 (*isol*)
Markham, K.R. *et al*, *Phytochemistry*, 1970, **9**, 2359 (*Rhamnosylglucoside*)
Beck, A.B. *et al*, *Aust. J. Chem.*, 1971, **24**, 1509 (*malonyl derivs*)
Imamura, H. *et al*, *Phytochemistry*, 1974, **13**, 757 (*Laminarabioside*)
Parthusarathy, M.R. *et al*, *Phytochemistry*, 1976, **15**, 1025 (*Rutinoside*)
Braz Filho, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1977, **40**, 236 (*isol*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Al-Ani, H.A.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1984, 2831 (*biosynth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 6th Ed., Van Nostrand-Reinhold, 1979, 736.

6-Hydroxy-7-methoxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran H-80191

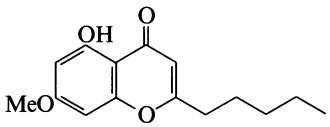


$C_{17}H_{22}O_3$ M 274.359
Metabolite of *Amaroucium multiplicatum*. Oil.

Sato, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 975 (*isol, pmr, cmr, synth*)

5-Hydroxy-7-methoxy-2-pentyl-4*H*-1-benzopyran-4-one H-80192

5-Hydroxy-7-methoxy-2-pentylchromone

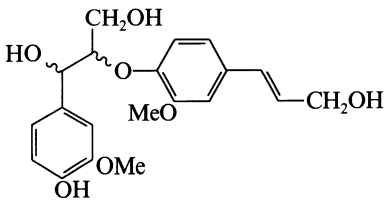


$C_{15}H_{18}O_4$ M 262.305
Constit. of *Zanthoxylum microcarpum* and *Z. valens*. Cryst. (EtOH). Mp 55-57°.

Jiménez, C. *et al*, *Phytochemistry*, 1989, **28**, 1992.

1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxy-1-propenyl)-2-methoxyphenoxy]-1,3-propanediol, 9CI H-80193

Guaiacylglycerol β-coniferyl ether
[1103-58-8]

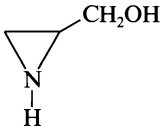


$C_{20}H_{24}O_7$ M 376.405
Prod. of lignin degradation. Isol. from wood of *Picea excelsa* and *Larix leptolepsis*. Syrup. $[\alpha]_D^{22}$ −6.7° (c, 0.53 in MeOH).

Freudenberg, K. *et al*, *Chem. Ber.*, 1955, **88**, 617, 626 (*synth, uv, ir*)
Nimz, H., *Chem. Ber.*, 1965, **98**, 533 (*isol*)
Miki, K. *et al*, *Phytochemistry*, 1980, **19**, 449 (*isol, pmr*)

2-(Hydroxymethyl)aziridine H-80194

2-Aziridinemethanol, 9CI
[88419-36-7]



C_3H_7NO M 73.094

(±)-*form*
Liq. $Bp_{0.005}$ 45° (bath) .

Trapensier, P.T. *et al*, *Chem. Heterocycl. Compd., Engl. Transl.*, 1983, **19**, 982 (*synth, pmr*)
Sehgal, R.K. *et al*, *J. Med. Chem.*, 1987, **30**, 1626 (*synth, pmr*)

3-Hydroxy-5-methylbenzaldehyde H-80195

Updated Entry replacing H-02277
*5-Hydroxy-*m*-tolualdehyde. 3,5-Cresotaldehyde.* m*-Cresol-5-aldehyde. 3-Formyl-5-methylphenol*
[60549-26-0]
$C_8H_8O_2$ M 136.150
Cryst. ($CHCl_3$). Mp 107-108°.

Me ether: [90674-26-3]. *3-Methoxy-5-methylbenzaldehyde*
$C_9H_{10}O_2$ M 150.177
Liq. Bp_{10} 95°. n_D^{20} 1.5475.

Brown, P.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 997 (*synth*)
Paisdor, B. *et al*, *Chem. Ber.*, 1988, **121**, 1307 (*deriv*)

5-(Hydroxymethyl)-1,2,3-benzenetriol H-80196

Updated Entry replacing H-02308
α,3,4,5-Tetrahydroxytoluene. 3,4,5-Trihydroxybenzyl alcohol. Gallyl alcohol
[68325-64-4]
$C_7H_8O_4$ M 156.138
Unstable, readily polymerises.

2-O-β-D-Glucopyranoside: ***MP-10***
$C_{13}H_{18}O_9$ M 318.280
Isol. from chestnut galls. Hygroscopic powder.

1′-O-(3,4,5-Trihydroxybenzoyl), 2-O-β-D-glucopyranoside: ***MP-2***
$C_{20}H_{22}O_{13}$ M 470.386
Isol. from chestnut galls. Needles. Mp 146-148°.

1,2,3-Tri-Me ether: 3,4,5-Trimethoxybenzyl alcohol
$C_{10}H_{14}O_4$ M 198.218
Viscous oil. Bp_{2-3} 160-165°.

1,2,3-Tri-Me ether, 1′-(3,5-dinitrobenzoyl): Mp 143-144°.

Rosemund, K.W. *et al*, *Ber.*, 1922, **55**, 2369 (*synth*)
Rosemund, K.W. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1927, **264**, 448; *CA*, **21**, 2886 (*synth*)
Drake, N.L. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 1204 (*synth*)
Ozawa, T. *et al*, *Agric. Biol. Chem.*, 1977, **41**, 1257 (*glycosides*)

2-(Hydroxymethyl)-1,4-butanediol, 9CI H-80197

Tris(hydroxymethyl)ethane
[6482-32-2]

$HOCH_2CH_2CH(CH_2OH)_2$

$C_5H_{12}O_3$ M 120.148
Liq.

Harnden, M.R. *et al*, *J. Med. Chem.*, 1987, **30**, 1636 (*synth, pmr*)

2-Hydroxy-3-methyl-2-butenenitrile, 9CI H-80198

1-Cyano-2-methyl-1-propen-1-ol

[116130-35-9]

$(H_3C)_2C{=}C(OH)CN$

C_5H_7NO M 97.116

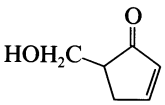
Enol form of 3-Methyl-2-oxobutanenitrile, (see 3-Methyl-2-oxobutanoic acid, M-80129). Isolable enol. Cryst. (pentane). Mp 30-32°.

Trifluoroacetyl: [116130-34-8].
$C_7H_6F_3NO_2$ M 193.125
Mp −2°. $Bp_{\sim 3}$ 40°.

Jaroszewski, J.W. *et al*, *J. Org. Chem.*, 1988, **53**, 4635 (*synth, uv, pmr, cmr, ir*)

5-(Hydroxymethyl)-2-cyclopenten-1-one, 9CI H-80199

[76909-98-3]

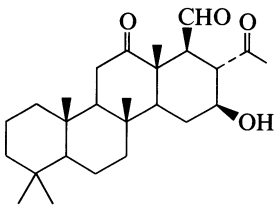


$C_6H_8O_2$ M 112.128

(±)-***form*** [110864-96-5]
Yellow oil.

Paulsen, H. *et al*, *Chem. Ber.*, 1981, **114**, 346.
Biggadike, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 549 (*synth, ir, pmr*)

16-Hydroxy-24-methyl-12,24-dioxo-25-scalaranal H-80200



$C_{26}H_{40}O_4$ M 416.600

16β-form

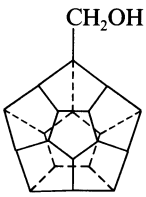
Ac: [116331-46-5]. *16β-Acetoxy-24-methyl-12,24-dioxo-25-scalaranal*
$C_{28}H_{42}O_5$ M 458.637
Constit. of *Carteriospongia flabellifera*. Cryst. Mp 227-229°. $[\alpha]_D$ +135° (c, 0.74 in $CHCl_3$).

Schmitz, F.J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 745.

(Hydroxymethyl)dodecahedrane H-80201

*Tetradecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene-1(2*H*)-methanol, 9CI. Dodecahedranemethanol*

[112896-32-9]



$C_{21}H_{22}O$ M 290.404
Solid. Mp >250°.

Paquette, L.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1303 (*synth, cmr*)
Weber, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5315 (*synth, pmr, cmr*)

2-Hydroxy-4,5-methylenedioxybenzoic acid H-80202

Updated Entry replacing H-60181

6-Hydroxy-1,3-benzodioxole-5-carboxylic acid, 9CI. 6-Hydroxypiperonylic acid, 8CI

$C_8H_6O_5$ M 182.132
Cryst. ($CHCl_3$). Mp 238° (216-217°).

Me ether: [7168-93-6]. *6-Methoxy-1,3-benzodioxole-5-carboxylic acid, 9CI. 6-Methoxy-*3,4*-methylenedioxybenzoic acid*
$C_9H_8O_5$ M 196.159
Needles ($CHCl_3$). Mp 153-153.2°.

Me ether, chloride:
$C_9H_7ClO_4$ M 214.605
Mp 118-121°.

Amide: [120781-07-9].
$C_8H_7NO_4$ M 181.148
Cryst. (C_6H_6). Mp 243-245°.

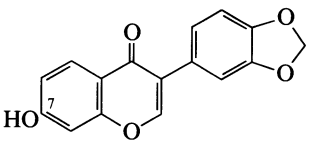
Dallacker, F. *et al*, *Justus Liebigs Ann. Chem.*, 1966, **694**, 98 (*deriv*)
Moron, J. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 130 (*synth*)
Stout, G.H. *et al*, *Tetrahedron*, 1969, **25**, 5295 (*deriv*)
Rall, G.J.H. *et al*, *Tetrahedron*, 1970, **26**, 5007 (*deriv*)
Dallacker, F. *et al*, *Z. Naturforsch., C*, 1978, **33**, 465 (*deriv*)
Sartori, G. *et al*, *Synthesis*, 1988, 783 (*synth, uv, ir, ms, pmr*)

7-Hydroxy-3′,4′-methylenedioxyisoflavone H-80203

Updated Entry replacing B-60006

*3-(1,3-Benzodioxol-5-yl)-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI. 7-Hydroxy-3-(3,4-methylenedioxyphenyl)chromone. Pseudobaptigenin. ψ-Baptigenin*

[90-29-9]



$C_{16}H_{10}O_5$ M 282.252

Isol. from *Baptisia* spp., *Cladrastis platycarpa*, *C. shikokiana*, several *Dalbergia* spp., *Maackia amurensis*, *Pisum sativum*, *Pterocarpus erinaceus*, *Trifolium hybridum* and *T. pratense*. Mp 296-298°. λ_{max} 226 (log ε 4.4), 248 sh and 294 nm (4.4) (MeOH).

Ac: Mp 173°.

O-*β-D-Glucopyranoside:* [63347-43-3]. ***Rothindin***
$C_{22}H_{20}O_{10}$ M 444.394
Isol. from *Rothia indica*, *Cladrastis platycarpa*, *C. shikokiana*, *Ononis spinosa* and *Trifolium pratense*. Needles (MeOH). Mp 236-237°. $[\alpha]_D^{32}$ −37.5° (Py).

O-*D-Glucosylrhamnoside:* ***ψ-Baptisin.*** *Pseudobaptisin*
$C_{22}H_{20}O_{10}$ M 444.394
Isol. from *B. tinctoria* and other *B.* sp. Cryst. + $3H_2O$. Mp 148-150° (resolidifies at 180-210° and remelts at 249-251°).

O-*Laminarabioside:*
$C_{28}H_{30}O_{15}$ M 606.536
Isol. from *Cladrastis platycarpa* and *C. shikokiana*. Tentative identification.

Me ether: [4253-04-7]. *7-Methoxy-3′,4′-methylenedioxyisoflavone. Pseudobaptigenin methyl ether*
$C_{17}H_{12}O_5$ M 296.279

Isol. from seeds of *Calopogonium mucunoides*. Mp 180-182°.

O-(*3-Methyl-2-butenyl*): ***Maximaisoflavone B***
$C_{21}H_{18}O_5$ M 350.370
Constit. of *Tephrosia maxima*. Cryst. (C_6H_6/pet. ether). Mp 132-133° (126-128°).

Schmidt, O. *et al*, *Monatsh. Chem.*, 1929, **53**, 454 (*isol, struct*)
Baker, W. *et al*, *J. Chem. Soc.*, 1953, 1582 (*synth*)
Kukla, A.S. *et al*, *Tetrahedron*, 1962, **18**, 1443 (*deriv*)
Bevan, C.W.L. *et al*, *J. Chem. Soc. C*, 1966, 509 (*pmr*)
Dhoubhadel, S.P. *et al*, *Indian J. Chem., Sect. B*, 1975, **52**, 440 (*synth*)
Nair, A.G.R. *et al*, *Indian J. Chem., Sect. B*, 1976, **14**, 801 (*Rothindin*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Schuda, P.F. *et al*, *J. Org. Chem.*, 1987, **52**, 1972 (*synth*)

Hydroxymethylenepropanedioic acid, 9CI H-80204

Updated Entry replacing H-02414
Hydroxymethylenemalonic acid, 8CI. Formylmalonic acid, 8CI

$$OHCCH(COOH)_2 \rightleftharpoons HOCH{=}C(COOH)_2$$

$C_4H_4O_5$ M 132.073

Enol-form [50850-50-5]
The free acid has not been isol.

Ba salt: Cryst. Mp 119°.

Mono-Me ester: Methyl hydrogen 2-formylmalonate
$C_5H_6O_5$ M 146.099
Prisms. Mp 38-40°.

Monobenzyl ester: Benzyl hydrogen 2-formylmalonate
$C_{11}H_{10}O_5$ M 222.197
Needles (hexane). Mp 54-56°.

Di-Et ester: [20734-18-3].
$C_8H_{12}O_5$ M 188.180
Liq. Bp_{12} 107-109°.

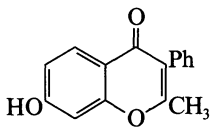
Aldo-form
The free acid has not been isol.

Di-Et ester, Di-Et acetal: [7251-32-3]. *Diethyl diethoxymethylmalonate*
$C_{12}H_{22}O_6$ M 262.302
Liq. Bp_{50} 70°.

v. Auers, K., *Justus Liebigs Ann. Chem.*, 1918, **415**, 169 (*ester, synth*)
Fuson, R.C. *et al*, *J. Org. Chem.*, 1946, **11**, 194 (*synth*)
Vinokurov, V.G. *et al*, *Zh. Fiz. Khim.*, 1968, **42**, 1052 (*spectra*)
Kabusz, S. *et al*, *Synthesis*, 1971, 312 (*acetal*)
Matrosov, E.I. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 191 (*spectra*)
Alaimo, R.J., *J. Heterocycl. Chem.*, 1973, **10**, 769 (*synth*)
Sato, M. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 665 (*monoesters*)

7-Hydroxy-2-methylisoflavone H-80205

*7-Hydroxy-2-methyl-3-phenyl-4*H*-1-benzopyran-4-one, 9CI*
[2859-88-3]



$C_{16}H_{12}O_3$ M 252.269

Isol. from roots of *Glycyrrhiza glabra*. Mp 240°.

Ac: [3211-63-0].
$C_{18}H_{14}O_4$ M 294.306
Isol. from *G. glabra*. Mp 161-162°.

Me ether: [19725-44-1]. *7-Methoxy-2-methylisoflavone*
$C_{17}H_{14}O_3$ M 266.296
Isol. from *G. glabra*. Mp 142-143°.

Woods, L.L. *et al*, *CA*, 1965, **62**, 6454f (*synth*)
Bhardwaj, D.K. *et al*, *Phytochemistry*, 1976, **15**, 352 (*isol*)

3-Hydroxymethyl-2-methylfuran H-80207

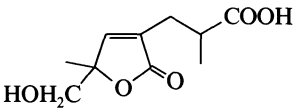
2-Methyl-3-furanmethanol
[5554-99-4]

$C_6H_8O_2$ M 112.128
Liq. Bp_7 70°. n_D^{16} 1.4876.

Ac:
$C_7H_{10}O_3$ M 142.154
Bp_{13} 77-79°.

Janda, M. *et al*, *Collect. Czech. Chem. Commun.*, 1964, **29**, 1731 (*deriv, synth*)
Valenta, M. *et al*, *Collect. Czech. Chem. Commun.*, 1966, **31**, 2410 (*synth*)
Scarpa, J.S. *et al*, *Helv. Chim. Acta*, 1966, **49**, 858 (*synth*)
Mann, J. *et al*, *Tetrahedron*, 1987, **43**, 2533 (*synth*)

3-(5-Hydroxymethyl-5-methyl-2-oxo-5*H*-furan-3-yl)-2-methylpropanoic acid H-80208

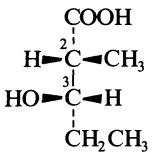


$C_{10}H_{14}O_5$ M 214.218
Constit. of *Crotalaria verrucosa*. Cryst. (C_6H_6). Mp 93°.

Suri, O.P. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 178 (*isol, pmr, cmr*)

3-Hydroxy-2-methylpentanoic acid, 9CI H-80209

Updated Entry replacing H-60192
3-Hydroxy-2-methylvaleric acid, 8CI
[28892-73-1]



(2*R*,3*S*)-*form*
Absolute configuration

$C_6H_{12}O_3$ M 132.159

(2R,3S)-form [77405-43-7]
Degradn. prod. of Mycobactin. Oil. $Bp_{0.1}$ 90-100°. $[\alpha]_D^{25}$ −14.8° (c, 4.3 in MeOH).

4-Bromophenacyl ester: Mp 89.5-90°. $[\alpha]_D^{18}$ −15° (c, 2.5 in MeOH).

3-Pentanoyl: ***Sitophilate***
$C_{11}H_{22}O_3$ M 202.293

Aggregation pheromone of granary weevil *Sitophilus granarius* (stereochem. of pheromone not detd.). Liq. $[\alpha]_D^{24}$ +3.0° (c, 1.5 in $CHCl_3$)(synthetic).

(2S,3S)-form

Me ester: Bp_5 69-70°. $[\alpha]_D^{23}$ +12.2° (c, 1.12 in $CHCl_3$).

(2RS,3SR)-form

Me ester: [67498-21-9].
$C_7H_{14}O_3$ M 146.186
Oil. Bp_4 68-70°.

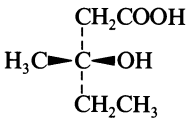
[60665-94-3, 67498-06-0, 78655-79-5, 78655-82-0, 84277-55-4, 100992-75-4]

Snow, G.A., *J. Chem. Soc.*, 1954, 4080 (*isol, synth*)
Snow, G.A., *Biochem. J.*, 1965, **94**, 160 (*abs config*)
Kirmse, W. *et al*, *Justus Liebigs Ann. Chem.*, 1976, 1333 (*synth*)
Aten, R.W. *et al*, *Synthesis*, 1978, 400 (*synth*)
Heathcock, C.H. *et al*, *J. Org. Chem.*, 1979, **44**, 4294 (*cmr*)
Mori, K. *et al*, *Tetrahedron*, 1986, **42**, 4685 (*synth, ir, pmr*)
Phillips, J.K. *et al*, *Tetrahedron Lett.*, 1987, **28**, 6145 (*Sitophilate*)
Chong, J.M., *Tetrahedron*, 1989, **45**, 623 (*Sitophilate*)

3-Hydroxy-3-methylpentanoic acid, 9CI H-80210

3-Hydroxy-3-methylvaleric acid. β-Methyl-β-ethylhydracrylic acid

[150-96-9]



(R)-form

$C_6H_{12}O_3$ M 132.159

(R)-form [36567-73-4]
Oil. $[\alpha]_D$ +1.07° (c, 2.25).

(±)-form
Isol. from Turkish tobacco leaves. Liq. Bp_{19} 142-144°.

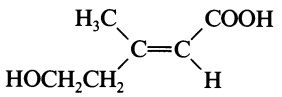
Et ester: [31033-23-5].
$C_8H_{16}O_3$ M 160.213
Liq. Bp_{19} 88-100°.

[114926-67-9]

Pocrowsky, A., *J. Prakt. Chem.*, 1900, **62**, 301 (*synth*)
Bohnsack, H. *et al*, *Ber.*, 1941, **74**, 1575 (*ester, synth*)
Papa, D. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 4441 (*synth*)
Kenyon, J. *et al*, *J. Chem. Soc.*, 1954, 2129 (*synth*)
Fukuzumi, T. *et al*, *Agric. Biol. Chem.*, 1966, **30**, 513 (*isol, ir*)
Seebach, P. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4763 (*synth, ir, pmr, cmr, ms*)

5-Hydroxy-3-methyl-2-pentenoic acid, 9CI H-80211

Δ^2-Anhydromevalonic acid



(E)-form

$C_6H_{10}O_3$ M 130.143
Metabolite of *Fusarium* and other fungi.

(E)-form [19710-84-0]
Component of Ferrirubin. Cryst. (C_6H_6). Mp 64-65°. pK_a 7.42.

Me ester: [35066-36-5].
$C_7H_{12}O_3$ M 144.170
Oil. Bp_9 115°.

(Z)-form [17880-06-7]
Component of Ferrirhodin. Prisms (C_6H_6). Mp 72-73°.

Me ester: [32775-50-1].
Oil. Bp_{15} 114°.

Lactone: [2381-87-5]. *5,6-Dihydro-4-methyl-2*H*-pyran-2-one, 9CI. Anhydromevalonolactone*
$C_6H_8O_2$ M 112.128
Key intermediate for synthesis of pheromones. Oil. Bp_{14} 118-120°, $Bp_{0.4}$ 65°. n_D^{21} 1.4840.

Cornforth, J.W. *et al*, *Biochem. J.*, 1958, **69**, 146 (*synth*)
Keller-Schierlein, W., *Helv. Chim. Acta*, 1963, **46**, 1920 (*isol*)
Dieckmann, H., *Arch. Microbiol.*, 1968, **62**, 322 (*isol*)
Keller-Schierlein, W. *et al*, *Helv. Chim. Acta*, 1972, **55**, 198 (*synth*)
Widmer, J. *et al*, *Helv. Chim. Acta*, 1974, **57**, 1904 (*synth*)
Bonadies, F. *et al*, *J. Org. Chem.*, 1984, **49**, 1647 (*synth, lactone*)

2-Hydroxymethyl-1,3-propanediol, 9CI H-80212

Tris(hydroxymethyl)methane

[4704-94-3]

$CH(CH_2OH)_3$

$C_4H_{10}O_3$ M 106.121
Chunky prisms (Me_2CO). Mp 67-68° (60-63°). $Bp_{2.5}$ 130-135° subl.

Tribenzoyl: [113967-50-3].
$C_{25}H_{22}O_6$ M 418.445
Needles (hexane). Mp 75-76°.

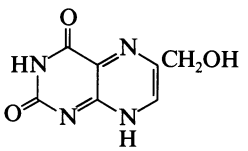
Tris(methanesulfonyl): Cryst. (EtOH aq.). Mp 83-84°.

Dekmizian, A.H. *et al*, *Synth. Commun.*, 1979, **9**, 431 (*synth, ir, pmr*)
Nielsen, A.T. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1981, **55**, 1393 (*synth, pmr, cmr*)
Latour, S. *et al*, *Synthesis*, 1987, 742 (*synth, ms, ir, pmr*)

6-(Hydroxymethyl)-2,4(1*H*,3*H*)pteridinedione H-80213

6-Hydroxymethyllumazine, 8CI

[10129-99-4]



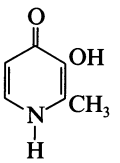
$C_7H_6N_4O_3$ M 194.149
Isol. from leaves of *Spinacia oleracea*. Mp 260-262° dec.

Sugiura, K. *et al*, *CA*, 1966, **65**, 15375, 20508 (*isol, uv, synth, struct*)

3-Hydroxy-2-methyl-4(1*H*)-pyridinone, 9CI H-80214

3,4-Dihydroxy-2-methylpyridine

[17184-19-9]



$C_6H_7NO_2$ M 125.127
Cryst. (H_2O). Mp 285-288°.

B,HCl: [17184-18-8].
Prisms (EtOAc/MeOH). Mp 185°.

O-*Ac:* [17184-20-2]. *3-Acetoxy-2-methyl-4(1*H*)-pyridinone*
$C_8H_9NO_3$ M 167.164
Cryst. (EtOAc). Mp 205-207°.

Me ether: [76015-11-7]. *3-Methoxy-2-methyl-4(1*H*)-pyridinone, 9CI*
$C_7H_9NO_2$ M 139.154
Cryst. (Me_2CO/MeOH). Mp 155-156°.

Benzyl ether: [61160-18-7].

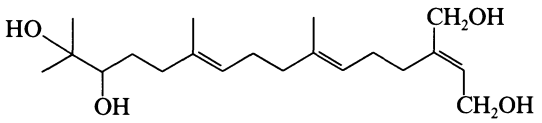
$C_{13}H_{13}NO_2$ M 215.251
Prisms (EtOH). Mp 162-163°.

O^3-β-D-Glucopyranosyl: [15266-34-9]. ***Innovanamine***
$C_{12}H_{17}NO_7$ M 287.269
Isol. from leaves of *Evodiopanax innovans*. Prisms + $2H_2O(H_2O)$. Mp 116-118°. $[\alpha]_D^{25}$ −61.6° (c, 10 in H_2O).

Yasue, M. *et al*, *Chem. Pharm. Bull.*, 1966, **14**, 1443 (*isol*)
Harris, R.L.N., *Aust. J. Chem.*, 1976, **29**, 1329 (*synth*)
Hwang, D.R. *et al*, *J. Pharm. Sci.*, 1980, **69**, 1074 (*synth*)

3-Hydroxymethyl-7,11,15-trimethyl-2,6,10-hexadecatriene-1,14,15-triol H-80215

[119877-40-6]



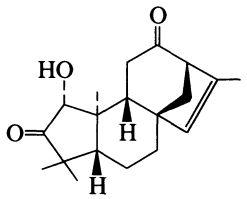
$C_{20}H_{36}O_4$ M 340.502
Constit. of *Tithonia pedunculata*. Oil. $[\alpha]_{241}$ +15.67° (c, 0.185 in MeOH).

Pérez, A.-L. *et al*, *Phytochemistry*, 1988, **27**, 3897.

ent-1β-Hydroxy-3-nor-15-beyerene-2,12-dione H-80216

Yucalexin B′-11

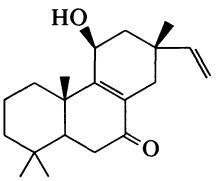
[119642-80-7]



$C_{19}H_{26}O_3$ M 302.413
Constit. of cassava roots (*Manihot esculenta*).

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

11-Hydroxy-20-nor-8,15-isopimaradien-7-one H-80217



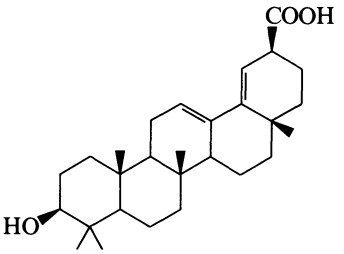
$C_{19}H_{28}O_2$ M 288.429

11β-form [83037-63-2]
Constit. of *Vellozia pusilla*. Cryst. (EtOAc/hexane). Mp 158-160°. $[\alpha]_D^{24}$ +116.1° (c, 0.58 in $CHCl_3$).

11-Ketone: [83037-65-4]. *20-Nor-8,15-isopimaradiene-7,11-dione*
$C_{19}H_{26}O_2$ M 286.413
Constit. of *V. pusilla*. Cryst. (hexane). Mp 80-82°.

Pinto, A.C. *et al*, *Phytochemistry*, 1988, **27**, 3913.

3-Hydroxy-30-nor-12,18-oleanadien-29-oic acid H-80218

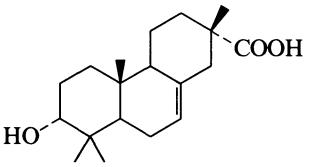


$C_{29}H_{44}O_3$ M 440.665

3β-form
Constit. of *Boussingaultia gracilis*.
Et ester: Cryst. (MeOH). Mp 107-108°.

Lin, H.-Y. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 797.

3-Hydroxy-16-nor-7-pimaren-15-oic acid H-80219



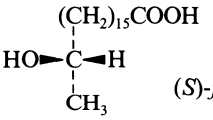
$C_{19}H_{30}O_3$ M 306.444

3α-form
Constit. of *Agathis vitiensis*. Cryst. (C_6H_6). Mp 208-210°. $[\alpha]_D^{18}$ −10° (c, 1.1 in $CHCl_3$).

Cambie, R.C. *et al*, *Phytochemistry*, 1989, **28**, 1675.

17-Hydroxyoctadecanoic acid H-80220

Updated Entry replacing H-02942
17-Hydroxystearic acid
[4552-19-6]



(*S*)-*form*

$C_{18}H_{36}O_3$ M 300.481
Occurs in beeswax (probably in an enantiomeric form).

(S)-form
Found as sophorose glycoside in *Torulopsis magnoliae*. Cryst. (Me_2CO). Mp 78-80°. $[\alpha]_D$ +4.4° (c, 7.9 in AcOH).

(±)-form
Mp 76.4-76.6°, Mp 81-81.4° (dimorph.).

Me ester: [2380-14-5].
$C_{19}H_{38}O_3$ M 314.507
Mp 52.0-52.5°, Mp 64.1-64.3° (dimorph.).

Bergström, S. *et al*, *Acta Chem. Scand.*, 1952, **6**, 1157 (*synth*)
Gorin, P.A.J. *et al*, *Can. J. Chem.*, 1961, **39**, 846 (*isol*)
Tulloch, A.P., *Chem. Phys. Lipids*, 1971, **6**, 235 (*isol*)
Hammerstrom, S. *et al*, *Anal. Biochem.*, 1973, **52**, 169 (*resoln*)
Tulloch, A.P. *et al*, *Org. Magn. Reson.*, 1978, **11**, 109 (*cmr*)

3-Hydroxy-28,13-oleananolide H-80221

Updated Entry replacing H-60200
$C_{30}H_{48}O_3$ M 456.707

(3β,13β)-form
Oleanolic lactone

Constit. of *Salvia lanigera*.

Ac: 3β-Acetoxy-28,13β-oleanolide
$C_{32}H_{50}O_4$ M 498.745
Constit. of *Hyptis mutabilis*. Needles ($CHCl_3$). Mp 282°.

Bellavista, V. *et al*, *Phytochemistry*, 1974, **13**, 289 (*isol*)
Al-Hazimi, H.M.G. *et al*, *Phytochemistry*, 1987, **26**, 1091 (*isol*)
Pereda-Miranda, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 996 (*isol*)

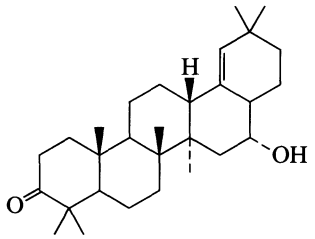
3-Hydroxy-12-oleanen-30-oic acid H-80222

$C_{30}H_{48}O_3$ M 456.707

3β-form [564-16-9]
11-*Deoxoglycyrrhetinic acid*
Cryst. (AOH). Isol. from roots of *Glycyrrhiza glabra*. Cryst. (AcOH). Mp 330°. $[\alpha]_D$ +148° (c, 0.473 in $CHCl_3$).

Canonica, L. *et al*, *Gazz. Chim. Ital.*, 1966, **96**, 833 (*isol, struct*)
Chakrabarti, P. *et al*, *J. Indian Chem. Soc.*, 1969, **46**, 626 (*synth*)

16-Hydroxy-18-oleanen-3-one H-80223



16α-*form*

$C_{30}H_{48}O_2$ M 440.708

16α-form
Constit. of *Schaefferia cuneifolia*.
Ac: Cryst. ($CHCl_3$). Mp 208-210°. $[\alpha]_D^{20}$ +31.5° (c, 0.14 in $CHCl_3$).

16β-form
Constit. of *S. cuneifolia*.
Ac: Cryst. ($CHCl_3$). Mp 210-212°. $[\alpha]_D^{20}$ +37° (c, 0.13 in $CHCl_3$).

Gonzalez, A.G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 567 (*isol, pmr, cmr*)

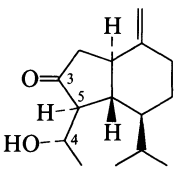
3-Hydroxy-12-oleanen-1-one H-80224

[120374-29-0]
$C_{30}H_{48}O_2$ M 440.708

3α-form
Constit. of *Randia dumetorum*. Needles (MeOH). Mp 268-270°. $[\alpha]_D$ +68°.

Murty, Y.L.N. *et al*, *Phytochemistry*, 1989, **28**, 276.

4-Hydroxy-10(15)-oplopen-3-one H-80225



$C_{15}H_{24}O_2$ M 236.353
Cadinane numbering used. Constit. of *Senecio mexicanus*. Cryst. Mp 100-102°. $[\alpha]_D$ −108° (c, 0.14 in $CHCl_3$).

Joseph-Nathan, P. *et al*, *Phytochemistry*, 1989, **28**, 2347 (*isol, pmr, cmr, cryst struct*)

3-Hydroxy-2-oxobutanoic acid H-80226

[1944-42-9]

$H_3CCH(OH)COCOOH$

$C_4H_6O_4$ M 118.089
Prod. by microorganisms e.g. *Aspergillus niger*. Isol. from berries of *Vaccinium vitis-idaea*. Component of cheese aroma.

Et ester, phenylhydrazone: Prisms. Mp 93-94°.

Virtanen, A.I. *et al*, *Acta Chem. Scand.*, 1955, **9**, 188 (*isol*)
Bowman, R.E. *et al*, *J. Chem. Soc.*, 1957, 1583 (*synth, deriv*)

4-Hydroxy-2-oxobutanoic acid H-80227

γ-Hydroxy-α-ketobutyric acid
[22136-38-5]

$HOCH_2CH_2COCOOH$

$C_4H_6O_4$ M 118.089
Isol. from fruits of *Vaccinium vitis-idaea* and from *V. oxycoccus*. Unstable, stabilised in frozen soln. at neutral pH.

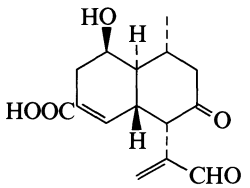
2,4-Dinitrophenylhydrazone: [22136-40-9].
Long yellow needles (EtOH). Mp 238-239°.

Lactone: Dihydro-2,3(2H,3H)-furandione
$C_4H_4O_3$ M 100.074
Needles. Mp 106-107°.

Virtanen, A.I. *et al*, *Acta Chem. Scand.*, 1955, **9**, 188 (*isol*)
Lane, A.S. *et al*, *Biochemistry*, 1969, **8**, 2958 (*synth, ir, uv*)

2-Hydroxy-12-oxo-4,11(13)-cadinadien-15-oic acid H-80228

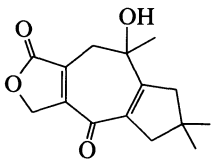
Panal
[115374-28-2]



$C_{15}H_{18}O_5$ M 278.304
Constit. of luminous mushroom *Panellus stipticus*. Amorph. solid. $[\alpha]_D$ −17° (c, 0.9 in MeOH).

Nakamura, H. *et al*, *Tetrahedron*, 1988, **44**, 1597 (*isol*)

3-Hydroxy-8-oxo-2(9),6-lactaradien-5,13-olide H-80229



$C_{15}H_{18}O_4$ M 262.305
Constit. of *Lactarius serobiculatus*.

Bosetti, A. *et al*, *Phytochemistry*, 1989, **28**, 1427.

3-Hydroxy-23-oxo-12-oleanen-28-oic acid H-80230

Updated Entry replacing H-03015
$C_{30}H_{46}O_4$ M 470.691

3β-form [639-14-5]
Gypsogenin

Cryst. (MeOH). Mp 274-276°. $[\alpha]_D$ +91° (EtOH).
▷ RK0178000.

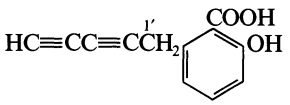
28-O-[[D-Xylopyranosyl(1→3)-O-6-deoxy-D-galactopyranosyl(1→2)]-6-deoxy-L-mannopyranoside], 3-O-[L-arabinopyranosyl(1→3)-O-(O-D-galactopyranosyl(1→4)-D-glucopyranosyl(1→4)-D-glucuronate)]: [15588-68-8]. ***Gypsoside***
$C_{80}H_{126}O_{44}$ M 1791.849
Constit. of *Gypsophila pacifica* and *G. paniculata*. $[\alpha]_D^{20}$ +47.5° (c, 3.4 in $CHCl_3$) (as Me ether).

3-O-α-D-Glucuronate: ***Vaccaroside***
$C_{36}H_{54}O_{10}$ M 646.817
Isol. from seeds of *Vaccaria segetalis*. Cryst. + $2H_2O$(EtOH). Mp 204-206°. $[\alpha]_D$ +16.5° (c, 1.75 in EtOH).

3-O-[D-Xylopyranosyl(1→4)-β-D-glucopyranosyl(1→3)-β-D-glucopyranosyl(1→4)-β-D-glucuronate]: ***Vacsegoside***
$C_{75}H_{118}O_{40}$ M 1659.733
Isol. from seeds of *V. segetalis*. Cryst. (MeOH/butanol). Mp 217-219°. $[\alpha]_D$ +7.5° (c, 3.16 in 30% MeOH aq.).

Ruzicka, L. *et al*, *Helv. Chim. Acta*, 1937, **20**, 299 (*isol*)
Vogel, A. *et al*, *Helv. Chim. Acta*, 1951, **34**, 2321 (*isol, struct*)
Kochetkov, N.K. *et al*, *Tetrahedron Lett.*, 1963, 477 (*Gypsoside*)
Abubakirov, N.K. *et al*, *Zh. Obshch. Khim.*, 1964, **34**, 1661 (*Vaccaroside*)
Amanmuradov, K. *et al*, *Khim. Prir. Soedin.*, 1965, **1**, 372; *cnc*, 292 (*Vacsegoside*)

2-Hydroxy-6-(2,4-pentadiynyl)benzoic acid, 9CI — H-80231



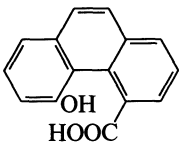
$C_{12}H_8O_3$ M 200.193

Me ether, Me ester: [4345-77-1]. ***Demethylfrutescin.*** *Desmethylfrutescin*
$C_{14}H_{12}O_3$ M 228.247
Isol. from roots of *Chrysanthemum frutescens*, *C. segetum* and *C. foeniculaceum*. Mp 68.5°.

Me ether, Me ester, 1'-acetoxy: ***Demethylfrutescin 1'-ylacetate.*** *Desmethylfrutescinol acetate*
$C_{16}H_{14}O_5$ M 286.284
Isol. from *C. frutescens* and *C. foeniculaceum*. Cryst. (Et_2O/pet. ether). $[\alpha]_D^{20}$ −1.6° (c, 1.9 in Et_2O). λ_{max} 284 nm (ε 3300)(Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 602; 1963, **26**, 226; 1964, **97**, 1179; 1966, **99**, 995 (*isol, uv, ir, struct, biosynth*)

5-Hydroxy-4-phenanthrenecarboxylic acid — H-80232



$C_{15}H_{10}O_3$ M 238.242

Lactone: 5H-Phenanthro[4,5-bcd]*pyran-5-one*
$C_{15}H_8O_2$ M 220.227
Pale-yellow needles (dioxan aq.). Mp 190°. Lactone ring opened with difficulty.

Me ether: 5-Methoxy-4-phenanthrenecarboxylic acid
$C_{16}H_{12}O_3$ M 252.269
Ppt. Mp 220°. Obt. only in low yield.

Gillis, R.G. *et al*, *Aust. J. Chem.*, 1989, **42**, 1007 (*synth, uv, pmr, ms*)

4-Hydroxy-1-phenyl-2-butyn-1-one — H-80233

3-Benzoyl-2-propyn-1-ol. 4-Hydroxy-2-butynophenone

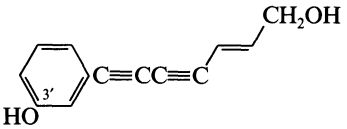
$PhCOC{\equiv}CCH_2OH$

$C_{10}H_8O_2$ M 160.172
Pale-yellow oil.

Obrecht, D., *Helv. Chim. Acta*, 1989, **72**, 447 (*synth, ir, pmr*)

7-(3-Hydroxyphenyl)-2-heptene-4,6-diyn-1-ol — H-80234

3-(7-Hydroxy-5-heptene-1,3-diynyl)phenol



$C_{13}H_{10}O_2$ M 198.221

(E)-form

3'-Ac: 7-(3-Acetoxyphenyl)-2-heptene-4,6-diyn-1-ol
$C_{15}H_{12}O_3$ M 240.258
Isol. from roots of *Coreopsis tinctoria*. Not obt. fully pure.

Di-Ac: 1-Acetoxy-7-(3-acetoxyphenyl)-2-heptene-4,6-diyne
$C_{17}H_{14}O_4$ M 282.295
Isol. from roots of *C. tinctoria*. Needles (Et_2O/pet. ether). Mp 90.5-91°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 1223, 2822 (*isol, uv, ir, pmr, struct, synth*)

6-Hydroxy-1-phenyl-2,4-hexadiyn-1-one, 9CI — H-80235

5-Benzoyl-2,4-pentadiyn-1-ol

[7358-89-6]

$PhCOC{\equiv}CC{\equiv}CCH_2OH$

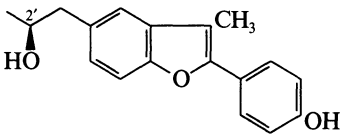
$C_{12}H_8O_2$ M 184.194
Isol. from *Lonas annua*. Cryst. (Et_2O/pet. ether). Mp 93°.

O-(3-Methyl-2-butenoyl): 1-(β-Methylcrotonoyloxy)-5-benzoyl-2,4-pentadiyne
$C_{17}H_{14}O_3$ M 266.296
Isol. from *L. annua*. Yellowish cryst. (pet. ether). Mp 36.5°.

[56558-91-9]

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2413 (*isol, uv, ir, pmr, synth*)
Fukumaru, T. *et al*, *Agric. Biol. Chem.*, 1975, **39**, 519 (*synth*)

2-(4-Hydroxyphenyl)-5-(2-Hydroxypropyl)-3-methylbenzofuran — H-80236



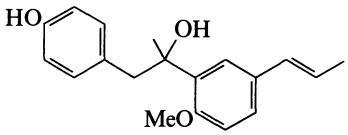
$C_{18}H_{18}O_3$ M 282.338
Constit. of *Krameria lanceolata*. Oil. $[\alpha]_D^{21}$ +9° (c, 0.3 in MeOH).

2'-Ketone: 2-(4-Hydroxyphenyl)-3-methyl-5-(2-oxopropyl)benzofuran
$C_{18}H_{16}O_3$ M 280.323
Constit. of *K. lanceolata*. Amorph.

Achenbach, H. *et al*, *Phytochemistry*, 1989, **28**, 1959.

1-(4-Hydroxyphenyl)-2-(2-methoxy-5-propenylphenyl)-2-propanol H-80237

4-[2-Hydroxy-2-(2-methoxy-5-propenylphenyl)propyl]phenol



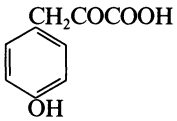
$C_{19}H_{22}O_3$ M 298.381

Constit. of *Krameria lanceolata*. Amorph. $[\alpha]_D^{21}$ +7° (c, 0.2 in MeOH).

Achenbach, H. *et al*, *Phytochemistry*, 1989, **28**, 1959.

3-(4-Hydroxyphenyl)-2-oxopropanoic acid H-80238

4-Hydroxy-α-oxobenzenepropanoic acid. p-*Hydroxyphenylpyruvic acid*



$C_9H_8O_4$ M 180.160

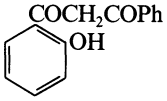
Isol. from cell cultures of *Aerobacter aerogenes* and *E. coli*. Also obt. from *Phlox* spp. and *Thuja plicata*. Cryst. Mp 218°.

Phenylhydrazone: Mp 161-162°.

Doy, C.H. *et al*, *Biochim. Biophys. Acta*, 1961, **50**, 495 (*isol, synth*)
Brandner, G. *et al*, *Acta Chem. Scand.*, 1964, **18**, 574 (*isol*)

1-(2-Hydroxyphenyl)-3-phenyl-1,3-propanedione H-80239

2′,β-Dihydroxychalcone



$C_{15}H_{12}O_3$ M 240.258

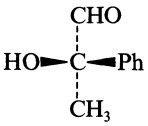
Enolised β-diketone. Constit. of *Primula pulverulenta*. Yellow prisms (MeOH). Mp 114-117°.

Wollenweber, E. *et al*, *Phytochemistry*, 1989, **28**, 295.

2-Hydroxy-2-phenylpropanal H-80240

α-Hydroxy-α-methylbenzeneacetaldehyde, 9CI. α-Methylmandelaldehyde, 8CI

[4361-50-6]



R-form

$C_9H_{10}O_2$ M 150.177

(R)-form

$Bp_{0.3}$ 108-110°, $Bp_{0.1}$ 90-110° (kugelrohr) . $[\alpha]_D^{20}$ +80.2° (c, 1.73 in $CHCl_3$, 31% opt. pure).

(±)-form

$Bp_{0.7}$ 116-120°.

Dimer: [21504-26-7]. *2,5-Dihydroxy-3,6-dimethyl-3,6-diphenyl-1,4-dioxan*

$C_{18}H_{20}O_4$ M 300.354

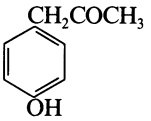
Mp <27°.

Russell, G.A. *et al*, *J. Org. Chem.*, 1969, **34**, 3618 (*synth*)
Oldenziel, O.H. *et al*, *Tetrahedron Lett.*, 1974, 167 (*synth*)
Hundscheid, F.J.A. *et al*, *Tetrahedron*, 1987, **43**, 5073 (*synth, ir, pmr*)

1-(4-Hydroxyphenyl)-2-propanone H-80241

p-*Hydroxyphenylacetone*

[770-39-8]



$C_9H_{10}O_2$ M 150.177

Yellowish oil or cryst. Mp 40°. Bp_{11} 168-170°.

Semicarbazone: Mp 212°.

Me ether: [122-84-9]. *1-(4-Methoxyphenyl)-2-propanone. Anisylacetone. Anisyl ketone*

$C_{10}H_{12}O_2$ M 164.204

Isol. from anise oil, fennel oil and oil of *Illicium verum*. Oil. Bp 261-265°.

Me ether, semicarbazone: [7306-38-9]. Mp 183-184° (174°).

Tardy, E., *Bull. Soc. Chim. Fr.*, 1897, 580, 660; 1902, 990 (*isol, deriv*)
Hoover, E.W. *et al*, *J. Org. Chem.*, 1947, **12**, 501 (*synth, deriv*)
Jones, D.D. *et al*, *J. Org. Chem.*, 1967, **32**, 1402 (*synth*)
Bricout, J., *Bull. Soc. Chim. Fr.*, 1974, 1901 (*isol, deriv*)
Franke, A. *et al*, *Helv. Chim. Acta*, 1975, **58**, 278 (*synth*)

3-(4-Hydroxyphenyl)-2-propenoic acid, 9CI H-80242

Updated Entry replacing H-50300

p-*Hydroxycinnamic acid, 8CI.* p-*Cumaric acid.* p-*Coumaric acid. Naringenic acid. Naringeninic acid*

[7400-08-0]

$C_9H_8O_3$ M 164.160

▷ GD9094000.

(E)-form [501-98-4]

Widespread in plants, e.g. peel of *Prunus serotina*, and from *Trifolium pratense*and *Daviesia latifolia*.. Cryst. + $1H_2O$ (cold H_2O), anhyd. cryst. (hot H_2O). Sol. Et_2O, hot EtOH, spar. sol. C_6H_6, insol. ligroin.

Me ester: [19367-38-5].

$C_{10}H_{10}O_3$ M 178.187

Needles (H_2O), tablets (EtOH). Mp 137°.

Et ester: [7362-39-2].

$C_{11}H_{12}O_3$ M 192.214

Mp 83°. $Bp_{0.08}$ 175-184°.

Glycoside: ***Pajaneelin***

Glycoside from peel of *Pajanelia rheedii*. Mp 237-239°. $[\alpha]_D^{30}$ −173°. Gives *p*-Coumaric acid and fructose on hydrol.

Me ester, glucoside: ***Linocinnamarin***

$C_{16}H_{20}O_8$ M 340.329

Glycoside from seeds of *Linum usitatissimum*. Fine needles (MeOH aq.). Mp 167° (anhyd.). $[\alpha]_D^{27}$ −73° (c, 1 in MeOH).

Triacontyl ester: ***Defuscin***

$C_{39}H_{68}O_3$ M 584.964

Constit. of *Dendrobium fuscescens*. Needles ($CHCl_3$/pet. ether). Mp 101°.

Me ether: [943-89-5]. *3-(4-Methoxyphenyl)-2-propenoic acid*

$C_{10}H_{10}O_3$ M 178.187

Isol. from oil of *Andropogon odoratus*, *Curcuma aromatica* and other plants. Needles (EtOH). Mp 170-172° (sinters).

Me ether, Et ester: [24393-56-4].
$C_{12}H_{14}O_3$ M 206.241
Major constit. of oil of *Kaempferia galanga*. Large prisms. Mp 49-50°.

O-(*3,7-Dimethyl-2,6-octadienyl*), *Me ester: Methyl* p-*geranyloxycinnamate*
$C_{20}H_{26}O_3$ M 314.424
Isol. from *Acronychia baueri*. Platelets (MeOH). Mp 65-67°.

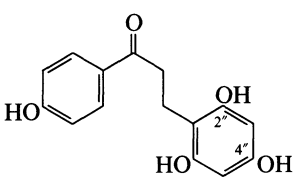
(***Z***)-***form*** [4501-31-9]
Found in *Larix sibirica* bark and *Miscanthus floridulus*. Cryst. (C_6H_6 or H_2O). Mp 134-134.5° dec. (subl. from 124°).

[830-09-1, 1929-30-2, 2979-06-8, 3943-97-3, 51507-22-3]

Zincke, T., *Justus Liebigs Ann. Chem.*, 1902, **322**, 224 (*isol*)
Ogawa, S., *Bull. Chem. Soc. Jpn.*, 1927, **2**, 25 (*isol*)
Klosterman, H.J. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 1229; 1955, **77**, 420 (*Linocinnamarin*)
U.S. Pat., 3 094 471, (1963); *CA*, **60**, 1655b (*isom*)
Prager, R.H. *et al*, *Aust. J. Chem.*, 1966, **19**, 451 (*Methyl p-*Geranyloxycinnamate)
Utsumi, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 426 (*cryst struct*)
Aulin-Erdtman, G. *et al*, *Acta Chem. Scand.*, 1968, **22**, 1187 (*props, uv*)
Hartley, R.D., *J. Chromatogr.*, 1975, **107**, 213 (*isom, gc*)
Talapatra, B. *et al*, *Phytochemistry*, 1989, **28**, 290 (*Defuscin*)

1-(4-Hydroxyphenyl)-3-(2,4,6-trihydroxyphenyl)-1-propanone H-80243

2,4,4′,6-Tetrahydroxydihydrochalcone



$C_{15}H_{14}O_5$ M 274.273

2″-Me ether: [119425-91-1]. *3-(2,4-Dihydroxy-6-methoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone.* ***Loureirin D***
$C_{16}H_{16}O_5$ M 288.299
Constit. of *Dracaena loueiri*. Powder (MeOH). Mp 176-178°.

2″,4″-Di-Me ether: 4-(2-Hydroxy-4,6-dimethoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone. ***Loureirin B***
$C_{17}H_{18}O_5$ M 302.326
Constit. of *D. loureiri*. Needles (MeOH). Mp 132-133°.

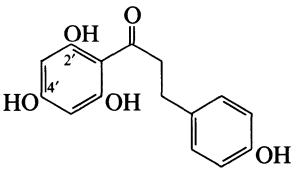
Meksuriyen, D. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1129 (*isol, pmr, cmr*)

3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone H-80244

Updated Entry replacing H-60219

2,4,4′,6-Tetrahydroxydihydrochalcone. Dihydronarigenin. Asebogenol. Phloretin. Phloretol

[60-82-2]



$C_{15}H_{14}O_5$ M 274.273
Occurs in apple (*Pyrus malus*) as glycosides and in leaves of lemon (*Citrus limon*). Needles (EtOH aq.). Insol. Et_2O. Mp ca. 262-264° dec.

2′-Glucoside: [60-81-1]. ***Phloridzin.*** *Phlorrhizin. Phlorhizin*
$C_{21}H_{24}O_6$ M 372.417
Occurs in *Micromelum teprocarpum*, in apple(*Malus*), *R.* spp., *Kalmia latifolia* and *Piperis japonica*. Produces glucosuria in man. Herbivore antifeedant. Needles. $[\alpha]_D^{18}$ −52.1° (EtOH aq.). Various Mp's, some double, recorded between 108° and 170°.
▷ UC2080000.

2′-Rhamnoside: [19253-17-9]. ***Glycyphyllin***
$C_{21}H_{24}O_9$ M 420.415
Isol. from leaves of *Smilax glycyphylla*. Large prisms (H_2O). Mp 175-180° dec.

4′-Me ether: [520-42-3]. *1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone.* ***Asebogenin.*** *Asebotol*
$C_{16}H_{16}O_5$ M 288.299
Found in *Piperis japonica*, *Rhododendron* spp. and *Pitryogramma calomelanos*. Cryst. (EtOH). Mp 168°.

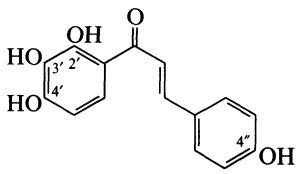
4′-Me ether, 2′-O-β-D-glucopyranoside: [11075-15-3]. ***Asebotin.*** *Asebotoside*
$C_{22}H_{26}O_6$ M 386.444
Constit. of *Andromeda japonica*, *R.* spp.,*K. latifolia* and *P. japonica*. Mp 148° (135-136°). $[\alpha]_D^{25}$ −46.2° (EtOH).

Eykman, J.F., *Ber.*, 1883, **16**, 2769 (*isol*)
Tamura, K., *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1936, **57**, 1141 (*synth, Asebogenin*)
Zemplén, R. *et al*, *Ber.*, 1942, **75**, 645, 1298 (*synth*)
Murakami, S., *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1955, **75**, 573, 603 (*isol*)
Batterham, T.J. *et al*, *Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Williams, A.H. *et al*, *Nature* (*London*), 1964, **202**, 824 (*isol, Glycyphyllin*)
Rice, G.L., *Allelopathy*, Academic Press, N.Y., 1974 (*deriv*)
King, B. *et al*, *Phytochemistry*, 1975, **14**, 1448 (*deriv*)
Mancini, S.D. *et al*, *J. Nat. Prod.* (*Lloydia*), 1979, **42**, 483 (*isol*)
Hutz, C. *et al*, *Z. Naturforsch.*, *C*, 1982, **37**, 337 (*isol*)

3-(4-Hydroxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, 9CI H-80245

Updated Entry replacing H-03269

2′,3′,4,4′-Tetrahydroxychalcone, 8CI. 4-Hydroxystyryl 2,3,4-trihydroxyphenyl ketone



$C_{15}H_{12}O_5$ M 272.257
Isol. from trunkwood of *Acacia auriculiformis*. Red-brown needles (EtOH aq.). Mp 225-225.5°.

4″-Me ether: 3-(4-Methoxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one. 2′,4,4′-Trihydroxy-3′-methoxychalcone. ***Kukulkanin B***
$C_{16}H_{14}O_5$ M 286.284
Constit. of *Mimosa tenuefolia*. Cryst. Mp 215°.

3′,4″-Di-Me ether: 1-(2,4-Dihydroxy-3-methoxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one. 2′,4′-Dihydroxy-3′,4-dimethoxychalcone. ***Kukulkanin A***
$C_{17}H_{16}O_5$ M 300.310
Constit. of *N. tenuefolia*. Cryst. Mp 172°.

Tetra-Me ether: Pale-yellow needles (EtOH). Mp 94°.

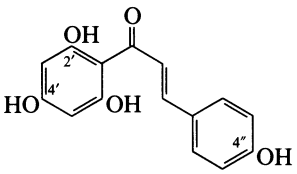
Russell, A. *et al*, *J. Chem. Soc.*, 1934, 220; 1937, 421 (*synth*, *uv*)
Geissman, T.A. *et al*, *J. Am. Chem. Soc.*, 1946, **68**, 697 (*synth*)
Drewes, S.E. *et al*, *Biochem. J.*, 1966, **98**, 493 (*isol*)

3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one, 9CI H-80246

Updated Entry replacing H-60220

2′,4,4′,6′-Tetrahydroxychalcone, 8CI. 4-Hydroxystyryl 2,4,6-trihydroxyphenyl ketone. ***Chalconaringenin***

[73692-50-9]



$C_{15}H_{12}O_5$ M 272.257

2′-Glucoside: [4547-85-7]. ***Isosalipurposide***
$C_{21}H_{22}O_{10}$ M 434.399
Isol. from *Salix purpurea*, *Paeonia trollioides*, *Dianthus caryophyllus*, *Aeschynanthus pariflorus* and *Asystasia gangetica*. Mp 172-174° (anhyd.). $[\alpha]_D$ −20° (EtOH).

2′-[O-Rhamnosyl(1→4)xyloside]: [82344-84-1].
$C_{26}H_{30}O_{13}$ M 550.515
Pigment from *Acacia dealbata*.

2′-Me ether, 4′-glucoside: [61826-89-9]. ***Helichrysin.*** *Dehydro-*p*-asebotin*
$C_{22}H_{24}O_{10}$ M 448.426
Constit. of the flowers of *Helichrysum* spp. and of *Gnaphalium affine*. Yellow cryst. (MeOH). Mp 246° dec. (199-200°). $[\alpha]_D^{30}$ −85.7° (MeOH).

4′-O-(3-Methyl-2-butenyl):
$C_{20}H_{20}O_5$ M 340.375
Constit. of *H. athrisciifolium*. Gum.

*4′,4″-Di-Me ether: 1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one. 2′,6′-Dihydroxy-*4,4′*-dimethoxychalcone.* ***Gymnogrammene***
$C_{17}H_{16}O_5$ M 300.310
Isol. from *Pitryogramma chrysophylla*. Red prisms (C_6H_6). Mp 156-157°.

2′,4′,4″-Tri-Me ether: [3420-72-2]. *3-(4-Hydroxyphenyl)-1-(2-hydroxy-4,6-dimethoxyphenyl)-2-propen-1-one. 2′-Hydroxy-*4,4′,6′*-trimethoxychalcone.* ***Flavokawin A***
$C_{18}H_{18}O_5$ M 314.337
Constit. of *Piper methysticum* and *Dahlia tenuicaulis*. Yellow needles (EtOH). Mp 113°.

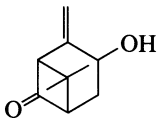
Tetra-Me ether: [25163-67-1].
$C_{19}H_{20}O_5$ M 328.364
Pale-yellow cryst. (EtOH aq.). Mp 119-121°.

*Dihydro, 6′-Me ether: 3-(4-Hydroxyphenyl)-1-(2,4-dihydroxy-6-methoxyphenyl)-1-propanone, 9CI. 2′,*4,4′*-Trihydroxy-6′-methoxydihydrochalcone*
$C_{16}H_{16}O_5$ M 288.299
Constit. of *Coptis japonica* var. *dissecta*. Needles (EtOH). Mp 195°.

Kostanecki, S. *et al*, *Ber.*, 1904, **37**, 792 (*synth*)
Mosimann, W. *et al*, *Ber.*, 1916, **49**, 1701 (*synth*)
Nilsson, M. *et al*, *Acta Chem. Scand.*, 1961, **15**, 211 (*Gymnogrammene*)
Guise, G.B. *et al*, *Aust. J. Chem.*, 1962, **15**, 314 (*isol*, *deriv*)
Mahanthy, P., *Indian J. Chem.*, 1965, **3**, 121 (*ir*)
Harborne, J.B. *et al*, *Phytochemistry*, 1966, **5**, 111 (*Isosalipurposide*)
Ramakrishnan, V.T. *et al*, *J. Org. Chem.*, 1970, **35**, 2901 (*synth*)
Aritomi, M. *et al*, *Chem. Pharm. Bull.*, 1974, **22**, 1800 (*Dehydroasebotin*)
Lam, J. *et al*, *Phytochemistry*, 1975, **14**, 1621 (*isol*, *deriv*)
Wright, W.G., *J. Chem. Soc.*, *Perkin Trans.* 1, 1976, 1819 (*Helichrysin*)
Duddeck, H. *et al*, *Phytochemistry*, 1978, **17**, 1369 (*pmr*)
Imperato, F., *Phytochemistry*, 1982, **21**, 480 (*rhamnosylxyloside*)
Bohlmann, F. *et al*, *Phytochemistry*, 1984, **23**, 1338 (*isol*)
Babber, S. *et al*, *Indian J. Chem.*, *Sect. B*, 1987, **26**, 797 (*synth*)
Mizuno, M. *et al*, *Phytochemistry*, 1987, **26**, 2071 (*deriv*)

2-Hydroxy-1(10)-pinen-5-one H-80247

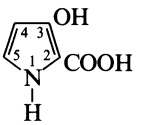
2-Hydroxy-5-oxo-β-pinene



$C_{10}H_{14}O_2$ M 166.219
Constit. of *Artemisia gypsacea*. Oil. $[\alpha]_D^{24}$ −24° (c, 1.2 in $CHCl_3$).

Rustaiyan, A. *et al*, *Phytochemistry*, 1989, **28**, 1535.

3-Hydroxy-1*H*-pyrrole-2-carboxylic acid H-80248



$C_5H_5NO_3$ M 127.099

Me ether, Me ester: [112373-17-8].
$C_7H_9NO_3$ M 155.153
Needles (EtOAc/hexane). Mp 112-114°.

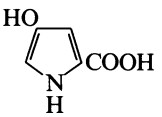
Me ether, Et ester:
$C_8H_{11}NO_3$ M 169.180
Cryst. by subl. Mp 94°.

Rapoport, H. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 635 (*synth*, *uv*)
Boger, D.L. *et al*, *J. Org. Chem.*, 1988, **53**, 1405 (*synth*, *pmr*, *cmr*, *ir*, *uv*, *ms*)

4-Hydroxy-1*H*-pyrrole-2-carboxylic acid H-80249

Updated Entry replacing H-10288

Hydroxyminaline



$C_5H_5NO_3$ M 127.099
Component of the molecule pectase found in *Penicillium* and *Aspergillus*. Grey-brown amorph. powder which cannot be recryst. or subl. Dec. readily in soln.

Me ether: 4-Methoxy-2-pyrrolecarboxylic acid
$C_6H_7NO_3$ M 141.126
Cryst. by subl. Mp 179-180°.

Me ether, Me ester:
$C_7H_9NO_3$ M 155.153
Cryst. (MeOH). Mp 85-86°.

Me ether, Et ester:
$C_8H_{11}NO_3$ M 169.180
Cryst. (C_6H_6). Mp 55-58°.

Minagawa, T., *Proc. Imp. Acad.* (*Tokyo*), 1945, **21**, 33, 37; *CA*, **47**, 151i, 152b (*isol*)
Kuhn, R. *et al*, *Chem. Ber.*, 1956, **89**, 1423 (*synth*, *uv*)
Rapoport, H. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 630 (*derivs*, *synth*, *uv*, *ir*)

4-Hydroxy-1*H*-pyrrole-3-carboxylic acid H-80250

$C_5H_5NO_3$ M 127.099

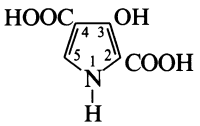
*Me ether: 4-Methoxy-1*H*-pyrrole-3-carboxylic acid*
$C_6H_7NO_3$ M 141.126
Cryst. (MeOH/C_6H_6). Mp 203-204°.

Me ether, Me ester:
$C_7H_9NO_3$ M 155.153
Cryst. by subl. Mp 115-117°.

Me ether, Et ester:
$C_8H_{11}NO_3$ M 169.180
Cryst. (C_6H_6 or by subl.). Mp 107-109°.

Rapoport, H. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 630 (*synth, uv, ir*)

3-Hydroxy-1*H*-pyrrole-2,4-dicarboxylic acid H-80251



$C_6H_5NO_5$ M 171.109

Di-Et ester:
$C_{10}H_{13}NO_5$ M 227.216
Cryst. (C_6H_6/hexane, MeOH aq. or by subl.). Mp 121°.

Me ether, Di-Et ester:
$C_{11}H_{15}NO_5$ M 241.243
Cryst. (C_6H_6/hexane or by subl.). Mp 83°.

N-*Me, Me ether, Di-Et ester:*
$C_{12}H_{17}NO_5$ M 255.270
Cryst. (hexane or by subl.). Mp 50°.

Rapoport, H. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 635 (*synth, ir, uv*)

3-Hydroxy-1*H*-pyrrole-2,5-dicarboxylic acid H-80252

$C_6H_5NO_5$ M 171.109

Me ether, 2-Me ester: [112373-15-6].
$C_8H_9NO_5$ M 199.163
Platelets (MeOH). Mp 182-184°.

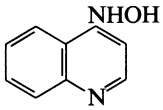
Me ether, Di-Me ester: [92144-13-3].
$C_9H_{11}NO_5$ M 213.190
Needles (MeOH). Mp 149.5-150.5°.

Boger, D.L. *et al*, *J. Org. Chem.*, 1988, **53**, 1405 (*synth, pmr, ir, ms*)

N-Hydroxy-4-quinolinamine, 9CI H-80253

4-Hydroxylaminoquinoline

[13442-05-2]



$C_9H_8N_2O$ M 160.175

B,HCl: [21626-47-1].
Mp 161-162°.

1-Oxide: [4637-56-3].
$C_9H_8N_2O_2$ M 176.174
Intermed. in carcinogenic activity of 4-aminoquinoline 1-oxide and related compds. Pale-brown needles or powder (MeOH). Mp 190° dec. Exists mainly as its hydroxyimino tautomer.

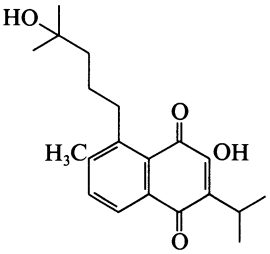
[1010-61-3]

Itai, T. *et al*, *Chem. Pharm. Bull.*, 1961, **9**, 87 (*oxide*)
Hamana, M. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1962, **84**, 42 (*synth*)
Kawazoe, Y. *et al*, *Tetrahedron*, 1980, **36**, 2933 (*uv, pmr, struct, oxide*)

4-Hydroxysapriparaquinone H-80254

3-Hydroxy-5-(4-hydroxy-4-methylpentyl)-6-methyl-2-(1-methylethyl)-1,4-naphthalenedione, 9CI. 3-Hydroxy-5-(4-hydroxy-4-methylpentyl)-2-isopropyl-6-methyl-1,4-naphthoquinone

[120278-25-3]



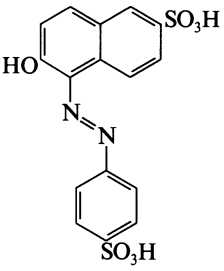
$C_{20}H_{26}O_4$ M 330.423
Constit. of *Salvia prionitis*. Cryst. Mp 61-62°. A 4,5-seco-5,10-friedoabietane.

Lin, L.-Z. *et al*, *Phytochemistry*, 1989, **28**, 177.

6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid, 9CI H-80255

1-(p-Sulfophenylazo)-2-naphthol-6-sulfonic acid. C.I. Food Yellow 3, 8CI. C.I. 15985

[5859-11-0]



$C_{16}H_{12}N_2O_7S_2$ M 408.412
Acid-base indicator. Orange cryst. Sol. H_2O, EtOH.

Di-Na salt: [2783-94-0]. *Sunset Yellow FCF*
Food dye. Sol. H_2O, v. sl. sol. EtOH.
▷ Mutagenic, carcinogenic, allergenic.

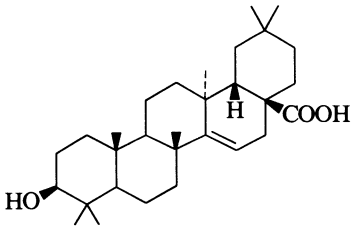
Ba salt: Deep orange-red, microscopic needles. V. sl. sol. H_2O.

Stein, C., *J. Assoc. Off. Agric. Chem.*, 1949, **32**, 672 (*synth, uv, anal*)
Berkman, Yu.P. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1956, **106**, 693 (*synth, use*)
Reich, G. *et al*, *Zh. Anal. Khim.*, 1960, **177**, 274 (*anal*)
Marmino, D.M., *J. Assoc. Off. Anal. Chem.*, 1974, **57**, 495 (*pmr*)
Saeva, F.D. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 5631 (*synth*)
Chudy, J. *et al*, *J. Chromatogr.*, 1978, **154**, 306 (*chromatog*)
Gelbcke, M. *et al*, *Anal. Lett. Sect. A, Sect. A*, 1980, **13**, 975 (*cmr*)
Broadbent, P. *et al*, *J. Chem. Res.* (*S*), 1980, 160 (*raman*)
Sugiura, T. *et al*, *J. Chem. Res.* (*S*), 1980, 164 (*ms, uv*)
Saint-Martin, P. *et al*, *Analusis*, 1987, **15**, LV (*hplc*)
Young, M. .L., *J. Assoc. Off. Anal. Chem.*, 1988, **71**, 458 (*tlc*)

3-Hydroxy-14-taraxeren-28-oic acid H-80256

Updated Entry replacing H-20250

3-Hydroxy-D-friedoolean-14-en-28-oic acid, 9CI



3β-*form*

$C_{30}H_{48}O_3$ M 456.707

3α-form

Epialeuritolic acid

Ac: ***Epiacetylaleuritolic acid***

$C_{32}H_{50}O_4$ M 498.745

Constit. of *Phytolacca acinosa*. Cryst. Mp 291-294°.

3β-form [26549-17-7] ***Aleuritolic acid.*** *Maprounic acid*

Constit. of *Aleuritus montana* and *Maprounea africana*. Cryst. ($CHCl_3$/MeOH). $[\alpha]_D^{20}$ +12.8° (c, 0.4 in Py).

Ac: [28937-85-1]. ***Acetylaleuritolic acid***

$C_{32}H_{50}O_4$ M 498.745

Constit. of *P. americana*. Cryst. Mp 300-302° dec., Mp 301-302°. $[\alpha]_D^{25}$ +23.1° (c, 0.6 in $CHCl_3$).

3-(4-Hydroxybenzoyl):

$C_{37}H_{52}O_5$ M 576.815

Constit. of *M. africana*. Cryst. Mp 308-311°. $[\alpha]_D^{20}$ +32.5° (c, 0.79 in Py).

Misra, D.R. *et al*, *Tetrahedron*, 1970, **26**, 3017 (*isol*)
Woo, W.S. *et al*, *Phytochemistry*, 1977, **16**, 1845 (*isol*)
Razdan, T.K. *et al*, *Phytochemistry*, 1982, **21**, 2339 (*isol*)
Wani, M.C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1983, **46**, 537 (*isol*)
McPhail, A.T. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 212 (*cryst struct, bibl*)

3-Hydroxy-11-triacontanone H-80257

[52656-91-4]

$H_3C(CH_2)_{18}CO(CH_2)_7CH(OH)CH_2CH_3$

$C_{30}H_{60}O_2$ M 452.803

Isol. from leaves of *Marsilea minuta*. Plates. Mp 102°. $[\alpha]_D^{25}$ −9° ($CHCl_3$).

Chakravarti, D. *et al*, *J. Indian Chem. Soc.*, 1974, **51**, 260.

7-Hydroxy-5-triacontanone H-80258

$H_3C(CH_2)_{22}CH(OH)CH_2CO(CH_2)_3CH_3$

$C_{30}H_{60}O_2$ M 452.803

Constit. of roots of *Costus speciosus*. Cryst. (Me_2CO/MeOH). Mp 81°.

Gupta, M.M. *et al*, *Phytochemistry*, 1981, **20**, 2553.

2-Hydroxytricosanoic acid, 9CI H-80259

[2718-37-8]

$H_3C(CH_2)_{20}CH(OH)COOH$

$C_{23}H_{46}O_3$ M 370.615

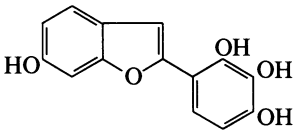
Present in cerebrosides.

[26632-12-2]

Downing, D.T., *Aust. J. Chem.*, 1961, **14**, 150 (*isol*)

6-Hydroxy-2-(2,3,4-trihydroxyphenyl)benzofuran H-80260

Updated Entry replacing P-02640



$C_{14}H_{10}O_5$ M 258.230

2′,3′-Di-Me ether: [74048-95-6]. *6-Hydroxy-2-(4-hydroxy-2,3-dimethoxyphenyl)benzofuran. 2-(4-Hydroxy-2,3-dimethoxyphenyl)-6-benzofuranol, 9CI.* ***Isopterofuran***

$C_{16}H_{14}O_5$ M 286.284

Isol. from leaves of *Coronilla emerus*.

2′,4′-Di-Me ether: [3784-75-6]. *2-(3-Hydroxy-2,4-dimethoxyphenyl)-6-benzofuranol, 9CI. 6-Hydroxy-2-(3-hydroxy-2,4-dimethoxyphenyl)benzofuran.* ***Pterofuran***

$C_{16}H_{14}O_5$ M 286.284

Constit. of the heartwood of *Pterocarpus indicus*. Needles (C_6H_6/EtOH). Mp 208-208.5°.

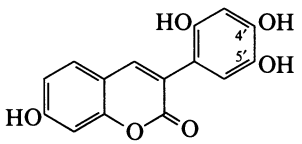
2′,4′-Di-Me ether, di-Ac: Needles (MeOH). Mp 135-136°.

Tetra-Me ether: Prisms (pet. ether). Mp 86-87°.

Cooke, R.G. *et al*, *Aust. J. Chem.*, 1964, **17**, 379 (*isol, struct*)
Cooke, R.G. *et al*, *Aust. J. Chem.*, 1969, **22**, 2395 (*synth*)
Duffley, R.P. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1977, 802 (*synth, pmr*)
Dewick, P.M. *et al*, *Phytochemistry*, 1980, **19**, 289 (*Isopterofuran*)

7-Hydroxy-3-(2,4,5-trihydroxyphenyl)-2*H*-1-benzopyran-2-one H-80261

7-Hydroxy-3-(2,4,5-trihydroxyphenyl)coumarin



$C_{15}H_{10}O_6$ M 286.240

4′,5′-Methylene ether: [54300-96-8]. *7-Hydroxy-3-(2-hydroxy-4,5-methylenedioxyphenyl)coumarin. 2′,7-Dihydroxy-4′,5′-methylenedioxy-3-phenylcoumarin*

$C_{16}H_{10}O_6$ M 298.251

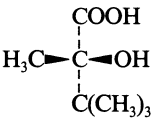
Isol. from heartwood of *Dalbergia oliveri*.

4′,5′-Methylene ether, di-Ac: Needles (EtOH aq.). Mp 195-196°.

Donnelly, D.M.X. *et al*, *Phytochemistry*, 1974, **13**, 2587 (*isol, uv, pmr, struct, synth*)

2-Hydroxy-2,3,3-trimethylbutanoic acid H-80262

2-tert-*Butyllactic acid*



(*R*)-*form*

$C_7H_{14}O_3$ M 146.186

(R)-form

Cryst. + $\frac{1}{2}H_2O$. $[\alpha]_D^{20}$ +1.4° (c, 8.36 in EtOH). Abs. config. has been uncertain – now prob. settled.

(S)-form

Needles + $\frac{1}{2}H_2O$ (pet. ether). Mp 67-69° (clears at 140°). $[\alpha]_D^{20}$ −1.5° (c, 9.83 in EtOH).

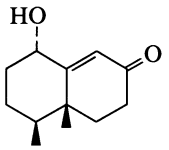
(±)-form

Mp 99-100° (clears at 140°).

Evans, R.J.D. *et al*, *J. Chem. Soc.*, 1963, 1506; 1965, 2553.
Eliel, E.L. *et al*, *Tetrahedron Lett.*, 1987, **28**, 4813 (*abs config, bibl*)

1-Hydroxy-11,12,13-trisnor-9-eremophilen-8-one H-80263

1-Hydroxyisoondetianone



$C_{12}H_{18}O_2$ M 194.273

(1α)-form

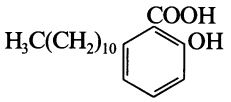
Constit. of *Ondetia linearis*. Oil. $[\alpha]_D^{24}$ +140° (c, 0.27 in $CHCl_3$).

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

2-Hydroxy-6-undecylbenzoic acid, 9CI H-80264

Anagigantic acid

[14155-32-9]



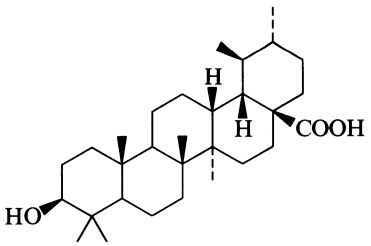
$C_{18}H_{28}O_3$ M 292.417

Isol. from the pericarp of *Anacardium giganteum* and from *Schistochila appendiculata*. Needles (hexane). Mp 81-82°.

K salt: [108049-75-8].
Mp 201-204° dec.

Sharma, P.V.K. *et al*, *Indian J. Chem.*, 1966, **4**, 99 (*isol, struct*)
Durrani, A.A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1979, 2069 (*synth, pmr, ir*)
Asakawa, Y. *et al*, *Phytochemistry*, 1987, **26**, 735 (*isol*)

3-Hydroxy-28-ursanoic acid H-80265



$C_{30}H_{50}O_3$ M 458.723

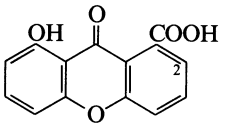
3β-form [120521-95-1]

Constit. of leaves of *Nerium oleander*. Cryst. ($CHCl_3$). Mp 150-152°. $[\alpha]_D$ +6.0° (c, 1 in $CHCl_3$).

Siddiqui, S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 57 (*isol, pmr, cmr*)

8-Hydroxyxanthone-1-carboxylic acid H-80266

8-Hydroxy-9-oxo-9H-xanthene-1-carboxylic acid, 9CI



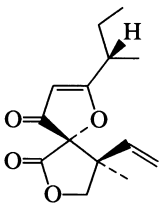
$C_{14}H_8O_5$ M 256.214

Me ester: [120461-93-0]. ***Vertixanthone***
$C_{15}H_{10}O_5$ M 270.241
Metab. of *Leptographium wageneri*. Yellow cryst. (EtOAc/pet. ether). Mp 152-154°.

2-Hydroxy, Me ester: [120461-95-2]. ***Hydroxyvertixanthone***
$C_{15}H_{10}O_6$ M 286.240
Metab. of *L. wageneri*. Yellow cryst. (Me_2CO). Mp 244-245°.

Ayer, W.A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 119 (*isol, ir, pmr, cmr*)

Hyperolactone H-80267



Relative configuration

$C_{14}H_{18}O_4$ M 250.294

Constit. of *Hypericum chinense*. Cryst. Mp 57°. $[\alpha]_D$ −228.93° (c, 0.13 in MeOH).

Tada, M. *et al*, *Chem. Lett.*, 1989, 683 (*cryst struct*)

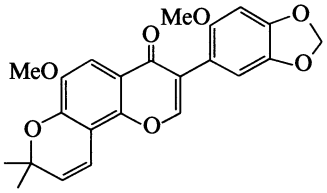
I

Ichthynone I-80001

Updated Entry replacing I-00016

*6-Methoxy-3-(6-methoxy-1,3-benzodioxol-5-yl)-8,8-dimethyl-4*H,*8*H-*benzo*[*1,2*-b:*3,4*b′]*dipyran-4-one, 9CI*

[24340-62-3]



$C_{23}H_{20}O_7$ M 408.407

Present in root bark of Jamaican Dogwood (*Piscidia erythrina* and from *Millettia rubininosa*). Fish poison. Rods (EtOH). Mp 203-204°.

Schwarz, J.S.P. *et al*, *Tetrahedron*, 1964, **20**, 1317 (*isol, uv, pmr, struct*)
Campbell, R.V.M. *et al*, *J. Chem. Soc. C*, 1969, 1787 (*isol, ms*)
Kirshnamurti, M. *et al*, *Indian J. Chem.*, 1972, **10**, 914 (*synth*)
Desai, H.K. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 291 (*isol*)

2-Icosanol I-80002

2-Eicosanol, 9CI

[4340-76-5]

$$H_3C(CH_2)_{17}CH(OH)CH_3$$

$C_{20}H_{42}O$ M 298.551

(+)-***form***

Isol. from bacterial lipids *Mycobacterium* spp. Needles (MeOH). $[\alpha]_D$ +4.2° ($CHCl_3$), $[\alpha]_D$ +6.79° (Et_2O).

[34019-45-9]

Anderson, R.J. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 10; 1937, **59**, 858 (*isol*)
Serck-Hanssen, K. *et al*, *CA*, 1954, **48**, 5071 (*synth*)
Elémadi, A.H. *et al*, *Bull. Soc. Chim. Biol.*, 1965, **47**, 2095 (*biosynth*)
Pearce, P.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 1655 (*synth*)

3-Icosene I-80003

3-Eicosene, 9CI

[42448-86-2]

$$H_3C(CH_2)_{15}CH{=}CHCH_2CH_3$$

$C_{20}H_{40}$ M 280.536

Isol. in small amt. from rose oil (*Rosa* spp.).

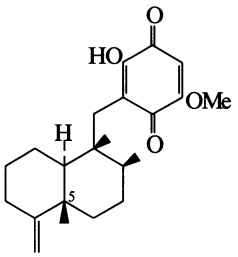
[74685-33-9]

Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1654.

Ilimaquinone I-80004

Updated Entry replacing I-70002

[71678-03-0]



Absolute configuration

$C_{22}H_{30}O_4$ M 358.477

Constit. of *Hippiospongia metachromia*. Cryst. (hexane). Mp 113-114°. $[\alpha]_D^{23}$ −23.2° (c, 1.12 in $CHCl_3$).

5-Epimer: [96806-31-4]. ***5-Epiilimaquinone***

$C_{22}H_{30}O_4$ M 358.477

Constit. of a *Fenestraspongia* sp.

O-*De-Me:* ***Smenoquinone***

$C_{21}H_{28}O_4$ M 344.450

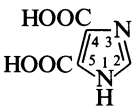
Constit. of *Smenospongia* sp. Cryst. Mp >350°.

Luibrand, R.T. *et al*, *Tetrahedron*, 1979, **35**, 609 (*isol*)
Carté, B. *et al*, *J. Org. Chem.*, 1985, **50**, 2785 (*Epiilimaquinone*)
Capon, R.J. *et al*, *J. Org. Chem.*, 1987, **52**, 5059 (*abs config*)
Kondracki, M.-L. *et al*, *Tetrahedron*, 1989, **45**, 1995 (*Smenoquinone*)

1*H*-Imidazole-4,5-dicarboxylic acid, 9CI I-80005

Updated Entry replacing I-00115

[570-22-9]



$C_5H_4N_2O_4$ M 156.098

Mp 288° dec.

▷ NI4760000.

Di-Me ester: [3304-70-9].
$C_7H_8N_2O_4$ M 184.151
Mp 200-203°.

Di-Et ester: [1080-79-1].
$C_9H_{12}N_2O_4$ M 212.205
Mp 151-152°.

Diamide: [83-39-6].
$C_5H_6N_4O_2$ M 154.128
Mp >360°.

Dihydrazide: [5423-20-1].
$C_5H_8N_6O_2$ M 184.157
Mp >375°.

Dinitrile: [1122-28-7]. *4,5-Dicyanoimidazole*
$C_5H_2N_4$ M 118.098
Cryst. (H_2O). Mp 172-173°.

1-Me: [19485-38-2].
$C_6H_6N_2O_4$ M 170.124
Cryst. Mp 259-260°.

1-Me, di-Me ester: [42545-22-2].

$C_8H_{10}N_2O_4$ M 198.178
Mp 46.5-47°.

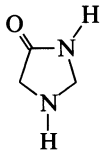
1-Me, diamide:
$C_6H_8N_4O_2$ M 168.155
Mp 268° (263-266°).

1-Me, dinitrile: [19485-35-9].
$C_6H_4N_4$ M 132.124
Cryst. Mp 87-89°.

Baxter, R.A. *et al*, *J. Chem. Soc.*, 1945, 232; 1947, 378 (*derivs*)
Castle, R.N. *et al*, *J. Org. Chem.*, 1958, **23**, 1534 (*deriv*)
Bauer, L. *et al*, *J. Heterocycl. Chem.*, 1964, **1**, 275 (*derivs*)
Yamada, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 1237 (*synth*)
Yasuda, N., *J. Heterocycl. Chem.*, 1985, **22**, 413 (*derivs*)
O'Connell, J.F. *et al*, *Synthesis*, 1988, 767 (*synth, pmr*)

4-Imidazolidinone I-80006

[1704-79-6]



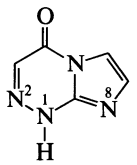
$C_3H_6N_2O$ M 86.093
Amorph. hygroscopic solid. Mp 64-67°.

3-Benzyl: [114981-12-3].
$C_{10}H_{12}N_2O$ M 176.218
Mp 164-169° (as hydrochloride).

Pfeiffer, U. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 993 (*synth, pmr, cmr, bibl*)

Imidazo[2,1-*c*][1,2,4]triazin-4(1*H*)-one I-80007

[59214-43-6]



$C_5H_4N_4O$ M 136.113
Mp 265° dec.

1-Me: [112298-51-8].
$C_6H_6N_4O$ M 150.140
Mp 159-160°.

8-Me: [112298-48-3].
$C_6H_6N_4O$ M 150.140
Mp 280-283°.

2-Me: [112298-52-9].
$C_6H_6N_4O$ M 150.140
Mp 247-250° dec. Zwitterionic.

Farràs, J. *et al*, *J. Org. Chem.*, 1988, **53**, 887 (*synth, pmr, cmr, ir*)

1,1′-Iminobis[3,3-dimethyl-2-butanone], 9CI I-80008

5-Aza-2,2,8,8-tetramethyl-3,7-nonanedione

[88686-46-8]

$$(H_3C)_3CCOCH_2NHCH_2COC(CH_3)_3$$

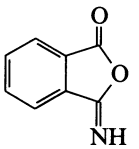
$C_{12}H_{23}NO_2$ M 213.319
Ligand. Cryst. by subl. Mp 61-62°.

Arduengo, A.J. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 627 (*synth, pmr, ir, use*)

3-Imino-1(3*H*)-isobenzofuranone, 9CI I-80009

3-Iminophthalide

[484-90-2]



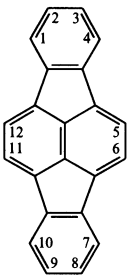
$C_8H_5NO_2$ M 147.133
Solid. Mp 112-116°. Exists largely as open chain tautomer.

Takeuchi, H. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2149 (*synth, pmr, ir*)

Indeno[1,2,3-*cd*]fluoranthene, 9CI, 8CI I-80010

Dibenz[a,g]*pyracyclene. Bis*-peri-*phenylenenaphthalene*

[193-43-1]



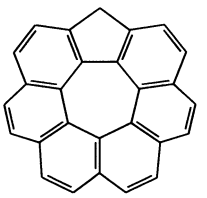
$C_{22}H_{12}$ M 276.337
Orange cryst. (C_6H_6). Mp 261-262°.

Dipicrate: Cryst. Mp 200°.

Clar, E. *et al*, *Nature (London)*, 1950, **166**, 1075 (*uv*)
Stubbs, H.W.D. *et al*, *J. Chem. Soc.*, 1951, 2936 (*synth, uv*)
Beaton, J.M. *et al*, *J. Chem. Soc.*, 1952, 3870.
Davies, A. *et al*, *J. Chem. Soc. B*, 1968, 1337 (*props*)
Elschenbroich, C. *et al*, *Helv. Chim. Acta*, 1970, **53**, 838 (*esr*)

Indeno[2,1,7,6-*ghij*]naphtho[2,1,8,7-*nopq*] pleiadene, 9CI I-80011

[114324-69-5]



$C_{27}H_{14}$ M 338.408
Yellow needles (C_6H_6). Mp 260° dec.

Yamamoto, K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3578 (*synth, ir, pmr, uv*)

1*H*-Indole-3-carboxylic acid I-80012

Updated Entry replacing I-00263

Indole-β-carboxylic acid

[771-50-6]

$C_9H_7NO_2$ M 161.160
Metab. of *Lasiodiplodia theobromae* and the marine algae *Undaria pinnatifida* and *Botryocladia leptopoda*. Mp 210-218° (198-200°).

Me ester: [942-24-5].
$C_{10}H_9NO_2$ M 175.187

Isol. from the red alga *B. leptopoda*. Mp 147-148° (140°). Probably an artifact.

Et ester: [776-41-0].
$C_{11}H_{11}NO_2$ M 189.213
Mp 122-124°.

Nitrile: [5457-28-3]. *3-Cyanoindole*
$C_9H_6N_2$ M 142.160
Mp 178°.

Nitrile, N-*Ac:*
$C_{11}H_8N_2O$ M 184.197
Mp 202°.

N-*COOEt, Et ester:*
$C_{14}H_{15}NO_4$ M 261.277
Cryst. (EtOH). Mp 102-104°.

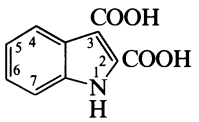
N-Me:
$C_{10}H_9NO_2$ M 175.187
Cryst. (2-propanol). Mp 212° (200-201° dec.).

N-*Benzyl:*
$C_{16}H_{13}NO_2$ M 251.284
Cryst. (EtOAc/hexane). Mp 198-204° (194-196°).

Kasparek, S. *et al*, *Can. J. Chem.*, 1966, **40**, 2805 (*synth*)
Katner, A.S., *Org. Prep. Proced. Int.*, 1970, **2**, 297 (*synth*)
Aldridge, D.C. *et al*, *J. Chem. Soc. C*, 1971, 1623 (*isol*)
Abe, H. *et al*, *Agric. Biol. Chem.*, 1972, **36**, 2259 (*isol, uv, ms*)
Kakehi, A. *et al*, *J. Org. Chem.*, 1976, **41**, 1570 (*esters*)
Bano, S. *et al*, *Planta Med.*, 1987, **53**, 117 (*isol, uv, pmr, cmr, ms, esters*)
Baiocchi, L. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1905 (*synth*)

1*H*-Indole-2,3-dicarboxylic acid I-80013

Updated Entry replacing I-00268



$C_{10}H_7NO_4$ M 205.170

3-Me ester: [34998-78-2].
$C_{11}H_9NO_4$ M 219.196
Cryst. (dioxan). Mp 254-255°.

Di-Me ester: [54781-93-0].
$C_{12}H_{11}NO_4$ M 233.223
Mp 112-112.5°.

N-*Me:*
$C_{11}H_9NO_4$ M 219.196
Cryst. (2-propanol). Mp 218° (208-209° dec.).

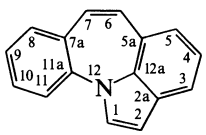
N-*Benzyl:*
$C_{17}H_{13}NO_4$ M 295.294
Cryst. + $1H_2O$ (EtOH). Mp 198° (194-196°).

N-*Ph:*
$C_{16}H_{11}NO_4$ M 281.267
Cryst. (MeOH). Mp 207-210° dec.

Huntress, E.H. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 419 (*synth*)
Baiocchi, L. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1905 (*synth, pmr*)

5*H*-Indolo[1,7-*ab*][1]benzazepine, 9CI I-80014

[202-01-7]



$C_{16}H_{11}N$ M 217.270

Yellow cryst. Mp 113-114°.

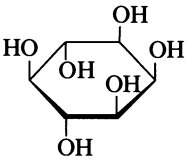
Hallberg, A. *et al*, *J. Heterocycl. Chem.*, 1981, **18**, 1255; 1983, **20**, 37; 1984, **21**, 1893 (*synth, uv, ms, pmr, cmr*)

myo-Inositol, 8CI I-80015

Updated Entry replacing I-10038

(*1α,2α,3α,4β,5α,6β*)-*Cyclohexanehexol.* meso-*Inositol. Dambose. Nucitol. 1,2,3,5/4,6-Inositol.* i-*Inositol. Inositol. Mesoinositol. Phaseomannitol. Myoinositol. Other proprietary names*

[87-89-8]



$C_6H_{12}O_6$ M 180.157

The most widely distributed member of the group of stereoisomers. Of common occurrence in plants and animals. Obt. comly. from phytic acid in corn steep liquor. Growth factor for animals and microorganisms. Toxic and lipotropic. Mp 225°. Opt. inactive (*meso-*).

*1,2-*O*-Cyclohexylidene:* [6763-47-9]. *1,2-*O*-Cyclohexylidene-*myo*-inositol*
$C_{12}H_{20}O_6$ M 260.286
Mp 179°.

*1,2:4,5-Di-*O*-isopropylidene:* [34379-30-1]. *1,2:4,5-Di-*O*-isopropylidene-*myo*-inositol*
$C_{12}H_{20}O_6$ M 260.286
Mp 174°.

*1,2:5,6-Di-*O*-cyclohexylidene:* [40773-57-7]. *1,2:5,6-Di-*O*-cyclohexylidene-*myo*-inositol*
$C_{18}H_{30}O_6$ M 342.431
Mp 133°, Mp 153-156°. $[\alpha]_D^{20}$ −7.4° (c, 0.5 in C_6H_6).

*1,4,5,6-Tetra-Ac: 1,2,5,6-Tetra-*O*-acetyl-*myo*-inositol*
$C_{14}H_{20}O_{10}$ M 348.306
Mp 100°.

1,2,3,4,6-Penta-Ac:
$C_{16}H_{22}O_{11}$ M 390.343
Mp 178°.

Hexa-Ac: [1254-38-2].
$C_{18}H_{24}O_{12}$ M 432.380
Mp 216-217°.

*Hexabenzoyl: 1,2,3,4,5,6-Hexa-*O*-benzoyl-*myo*-inositol*
$C_{48}H_{36}O_{12}$ M 804.805
Mp 258°.

Hexa(3-pyridinecarboxyl): [6556-11-2]. ***Inositol nicotinate*, BAN, INN.** *Inositol niacinate, USAN. Hexanicotinoylinositol. Hexopal. Mesonex. Lipoflavonoid. Numerous proprietary names*
$C_{42}H_{30}N_6O_{12}$ M 810.732
Peripheral vasodilator, antilipidaemic agent. Mp 254-255°.
▷ NM7535400.

1-Phosphate: [573-35-3].
$C_6H_{11}O_9P$ M 258.121
Wheat bran phytase hydrol. prod. of sodium phytate. Mp 195-197° dec.

1-Phosphate, biscyclohexylammonium salt: Mp 202-204°. $[\alpha]_D^{20}$ +3.4° (c, 1.0 in H_2O).

1,4-Diphosphate:
$C_6H_{10}O_{12}P_2$ M 336.085
Mp 206-207° (as bis(cyclohexylammonium) salt).

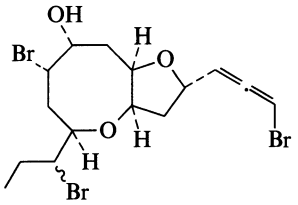
Hexaphosphate: [83-86-3]. ***Phytic acid.*** *Fytic acid, INN. Alkalovert*
$C_6H_{18}O_{24}P_6$ M 660.036
Complexing agent for the removal of traces of heavy metals; therapeutic hypocalcaemic agent, freq. employed as nona-Na salt (Sodium phytate, USAN). Straw-coloured syrup.
▷ NM7525000.

[7205-52-9, 17211-15-3]

Badgett, C.O. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 2907 (*nicotinate*)
Biochem. Prep., 1952, **2**, 65.
Angyal, S.J. *et al*, *Adv. Carbohydr. Chem.*, 1959, **14**, 135 (*rev*)
Angyal, S.J. *et al*, *J. Chem. Soc.*, 1961, 4116, 4122, 4718.
Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985, no. 280 (*bibl*)
Shvets, V.I. *et al*, *Tetrahedron*, 1973, **29**, 331.
Isbrandt, L.R. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 3144.
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 1056, 7877, 9243.
Wells, W.W., *Kirk-Othmer Encycl. Chem. Technol.*, 3*rd Ed.*, 1978-1984, *Wiley, NY*, 3rd Ed., Wiley, N.Y., 1983, **24**, 50 (*rev*)
Bleasdale, J.E. *et al*, Eds., *Inositol and Phosphoinositides:Metabolism and Regulation*, Humane Press,Clifton, N.J., 1985 (*book*)
Holub, B.J., *Annu. Rev. Nutr.*, 1986, **6**, 563 (*rev*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 540, 588, 8197 (*synonyms*)

Intricata bromoallene I-80016

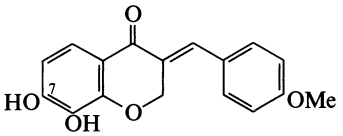
[123297-18-7]



$C_{15}H_{21}Br_3O_3$ M 489.041
Constit. of *Laurencia intricata*. Oil. $[\alpha]_D^{21}$ +95.8° (c, 0.6 in $CHCl_3$).

Suzuki, M. *et al*, *Phytochemistry*, 1989, **28**, 2145 (*isol, pmr, cmr*)

Intricatinol I-80017



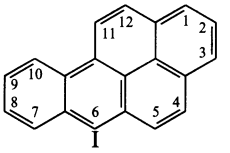
$C_{17}H_{14}O_5$ M 298.295
Constit. of *Hoffmanosseggia intricata*. Yellow needles (MeOH aq.). Mp 196-198°.

7-Me ether: ***Intricatin***
$C_{18}H_{16}O_5$ M 312.321
Constit. of *H. intricata*. Yellow cryst. (MeOH aq.). Mp 157-159°.

Wall, M.E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **28**, 774 (*isol, pmr*)

6-Iodobenzo[*a*]pyrene I-80018

[39000-82-3]

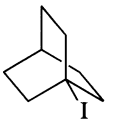


$C_{20}H_{11}I$ M 378.211
Cryst. Mp 214-215°.

Tye, R. *et al*, *Anal. Chem.*, 1955, **27**, 248 (*synth, uv*)
Johnson, M.D. *et al*, *Nature* (*London*), 1973, **241**, 271 (*synth, pmr*)

1-Iodobicyclo[2.2.2]octane I-80019

[931-98-6]

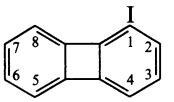


$C_8H_{13}I$ M 236.095
Cryst. (MeOH). Mp 27.5-28.5°.

Suzuki, Z. *et al*, *J. Org. Chem.*, 1967, **32**, 31 (*synth*)
Adcock, W. *et al*, *Organometallics*, 1987, **6**, 155 (*synth*)

1-Iodobiphenylene I-80020

[17557-56-1]



$C_{12}H_7I$ M 278.092
Yellow prisms (hexane). Mp 44-45°.

2,4,7-Trinitrofluorenone complex: [17557-55-0]. Deep red leaflets (C_6H_6/MeOH). Mp 177-179°.

Barton, J.W. *et al*, *J. Chem. Soc. C*, 1968, 28 (*synth, uv*)
Boulton, A.J. *et al*, *J. Chem. Soc. C*, 1968, 328 (*synth*)

2-Iodobiphenylene I-80021

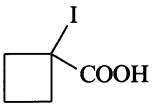
[96694-91-6]
$C_{12}H_7I$ M 278.092
Pale yellow plates (MeOH). Mp 64.5-65.5°.

2,4,7-Trinitrofluorenone complex: Scarlet cryst. (EtOH/AcOH). Mp 132.5-134°.

Baker, W. *et al*, *J. Chem. Soc.*, 1958, 2666 (*synth, uv*)
Cracknell, M.E. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1985, 115.

1-Iodocyclobutanecarboxylic acid I-80022

[115420-18-3]



$C_5H_7IO_2$ M 226.014
Cryst. (Et_2O/pentane). Mp 48-50°.

Renaud, P. *et al*, *J. Org. Chem.*, 1988, **53**, 3745 (*synth, pmr, cmr*)

5-Iodo-4,4-dimethyl-1-pentene, 9CI I-80023

[95106-80-2]

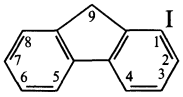
$H_2C{=}CHCH_2C(CH_3)_2CH_2I$

$C_7H_{13}I$ M 224.084
Light yellow oil. Bp_{12} 56-57°.

Pattenden, G. *et al*, *Tetrahedron*, 1987, **43**, 5637 (*synth, ir, pmr*)

1-Iodo-9*H*-fluorene I-80024

[54366-33-5]



$C_{13}H_9I$ M 292.119
Mp 40-42°.

Minabe, M. *et al*, *J. Org. Chem.*, 1975, **40**, 1298 (*synth*)

2-Iodo-9*H*-fluorene I-80025

[2523-42-4]

$C_{13}H_9I$ M 292.119
Cryst. (EtOH). Mp 129°.

Barnett, M.D. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 4583 (*synth*)
Chardonnens, L. *et al*, *Helv. Chim. Acta*, 1969, **52**, 1091 (*synth*)
Shapiro, M.J., *J. Org. Chem.*, 1978, **43**, 3769 (*cmr*)

9-Iodo-9*H*-fluorene I-80026

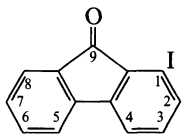
[64421-01-8]

$C_{13}H_9I$ M 292.119
Light yellow cryst. (pet. ether). Mp 148-149° dec.
Unstable, readily loses iodine.

Dickinson, J.D. *et al*, *J. Chem. Soc.*, 1959, 2337 (*synth*)
Shapiro, M.J. *et al*, *J. Org. Chem.*, 1978, **43**, 3769 (*synth, pmr, cmr*)
Hauser, A. *et al*, *J. Prakt. Chem.*, 1985, **327**, 433 (*pmr, cmr*)

1-Iodo-9*H*-fluoren-9-one I-80027

[52086-21-2]



$C_{13}H_7IO$ M 306.102
Yellow needles (EtOH). Mp 146.5-147°.

Huntress, E.H. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 2845 (*synth*)
Hojo, M. *et al*, *J. Org. Chem.*, 1985, **50**, 1478.

2-Iodo-9*H*-fluoren-9-one I-80028

[3096-46-6]

$C_{13}H_7IO$ M 306.102
Bright yellow needles (EtOH). Mp 152-153°.

Barnett, M.D. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 4583 (*synth*)
Chardonnens, L. *et al*, *Helv. Chim. Acta*, 1967, **52**, 1091 (*synth*)
Fukuyama, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 4363 (*synth*)

3-Iodo-9*H*-fluoren-9-one I-80029

[19063-38-8]

$C_{13}H_7IO$ M 306.102
Yellow needles (EtOH). Mp 160.5-161°.

Harget, A.J. *et al*, *J. Chem. Soc. B*, 1968, 214 (*synth*)

4-Iodo-9*H*-fluoren-9-one I-80030

[883-33-0]

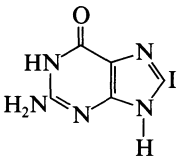
$C_{13}H_7IO$ M 306.102
Yellow prisms (EtOH). Mp 121-122°.

Newman, M.S. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 5601 (*synth*)

8-Iodoguanine, 8CI I-80031

*2-Amino-1,7-dihydro-8-iodo-6*H*-purin-6-one. 2-Amino-6-hydroxy-8-iodopurine*

[19690-21-2]



$C_5H_4IN_5O$ M 277.024
B,HCl: [21323-46-6].
Cryst.

Lipkin, D. *et al*, *J. Biol. Chem.*, 1963, **238**, 6 (*synth*)
Holmes, R.E. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1242 (*synth*)
Koda, R.T. *et al*, *J. Polym. Sci.*, 1968, **57**, 2056 (*synth*)

7-Iodo-1,3-heptadiene I-80032

$H_2C{=}CHCH{=}CHCH_2CH_2CH_2I$

$C_7H_{11}I$ M 222.068

(E)-form
Liq. $Bp_{3.5}$ 55-60°.

Vedejs, E. *et al*, *J. Org. Chem.*, 1988, **53**, 2220 (*synth, ir, pmr*)

Iodomethanol I-80033

[50398-30-6]

ICH_2OH

CH_3IO M 157.939

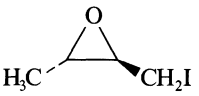
Ac: [13398-11-3].
$C_3H_5IO_2$ M 199.976
Alkylating agent. Oil. d_4^{20} 1.953. Bp_{14} 49-50°. n_D^{20} 1.5130.
▷ Lachrymator.

Benzoyl: [13943-33-4].
$C_8H_7IO_2$ M 262.047
Cryst. (pet. ether). Mp 32-33°.

4-Methylbenzenesulfonyl: [117184-52-8].
$C_8H_9IO_3S$ M 312.128
Oil. $Bp_{0.2}$ 115-120°.

Renshaw, R.R. *et al*, *J. Am. Chem. Soc.*, 1925, **47**, 2989 (*acetate*)
Euranto, E.K. *et al*, *Acta Chem. Scand.*, 1966, **20**, 1966 (*acetate*)
Wittig, G. *et al*, *Justus Liebigs Ann. Chem.*, 1967, **702**, 24 (*benzoate*)
Hahn, R.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5783 (*tosylate, synth, pmr, cmr*)

2-Iodomethyl-3-methyloxirane I-80034



C_4H_7IO M 198.003

(2RS,3SR)-form

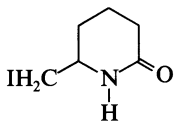
(±)-trans-form
$Bp_{4.2}$ 39-40°.
Evans, R.D. *et al*, *Synthesis*, 1988, 862 (*synth, pmr*)

2-(Iodomethyl)naphthalene I-80035

[24515-49-9]
$C_{11}H_9I$ M 268.097
Cryst. (EtOH). Mp 79° (72-73.5°). Unstable.
Daub, G.H. *et al*, *J. Org. Chem.*, 1954, **19**, 1571 (*synth*)
Bilgèr, C. *et al*, *Synthesis*, 1988, 902 (*synth*)

6-(Iodomethyl)-2-piperidinone, 9CI I-80036

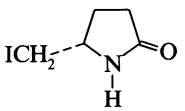
[100556-63-6]



$C_6H_{10}INO$ M 239.056
(±)-*form*
Cryst. (Et_2O/hexane). Mp 157-158°.
Knapp, S. *et al*, *J. Org. Chem.*, 1988, **53**, 4006 (*synth, ir, pmr*)

5-(Iodomethyl)-2-pyrrolidinone, 9CI I-80037

[5831-75-4]



(*S*)-*form*

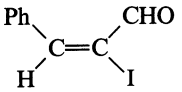
C_5H_8INO M 225.029
(*S*)-*form* [29266-73-7]
L-form
Cryst. (EtOAc). Mp 86-87°. $[\alpha]_D$ −55° (c, 1.24 in EtOH).
N-*Ac:*
$C_7H_{10}INO_2$ M 267.066
Yellowish oil. $[\alpha]_D$ −82° (c, 3.6 in EtOH).
(±)-*form*
Cryst. (Et_2O/hexane). Mp 68-70°.
Hardegger, E. *et al*, *Helv. Chim. Acta*, 1955, **38**, 312.
Molin-Case, J.A. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 4728 (*cryst struct, abs config*)
Knapp, S. *et al*, *J. Org. Chem.*, 1988, **53**, 4006 (*synth, ir, pmr*)

2-Iodo-6-nitrobenzaldehyde I-80038

[117847-41-3]
$C_7H_4INO_3$ M 277.018
Cryst. (EtOH). Mp 120-122°.
Hewgill, F.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1305 (*synth, ir, pmr*)

2-Iodo-3-phenyl-2-propenal, 9CI I-80039

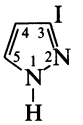
α-*Iodocinnamaldehyde*



C_9H_7IO M 258.058
(*E*)-*form* [52741-39-6]
Yellow prisms (EtOH). Mp 89° (85-86°).
[116544-98-0]
Coulomb, F. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 3352 (*synth, ir, pmr*)
Suzuki, H. *et al*, *Synthesis*, 1988, 236 (*synth, ir, pmr, ms*)

3(5)-Iodopyrazole, 8CI I-80040

[4522-35-4]



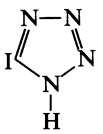
$C_3H_3IN_2$ M 193.975
Needles (H_2O). Mp 72-73°.
1-Me: [92525-10-5]. *3-Iodo-1-methylpyrazole, 9CI*
$C_4H_5IN_2$ M 208.001
Bp_{11} 100-102°.
2-Me: [34091-51-5]. *5-Iodo-1-methylpyrazole, 9CI*
$C_4H_5IN_2$ M 208.001
Cryst. (ligroin). Mp 76-76.5°. Sublimes at 50°/2mm.
Reimlinger, H.K. *et al*, *Chem. Ber.*, 1962, **94**, 1036 (*synth*)
Vasilevskii, S.F. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1971, 1655 (*synth, deriv*)
Effenberger, F. *et al*, *J. Org. Chem.*, 1984, **49**, 4687 (*synth, pmr, derivs*)

4-Iodopyrazole, 9CI I-80041

[3469-69-0]
$C_3H_3IN_2$ M 193.975
Needles (cyclohexane). Mp 109-110°.
1-Me: [39806-90-1]. *4-Iodo-1-methylpyrazole, 9CI*
$C_4H_5IN_2$ M 208.001
Crysts. (C_6H_6) or prisms (hexane), with odour like that of collidine. Mp 64-65°. Bp_{15} 101-105°.
Hüttel, R. *et al*, *Justus Liebigs Ann. Chem.*, 1955, **593**, 200 (*synth, deriv*)
Elguero, J. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 3727, 3744 (*pmr, uv*)
Vasilevskii, S.F. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1972, 2453 (*deriv*)
Rydberg, V. *et al*, *J. Chromatogr.*, 1972, **64**, 170 (*glc, ms*)
Liljefors, S. *et al*, *Chem. Scr.*, 1980, **15**, 102 (*synth, deriv*)
Cabildo, P. *et al*, *Org. Magn. Reson.*, 1984, **22**, 603 (*cmr*)

5-Iodo-1*H*-tetrazole, 9CI, 8CI I-80042

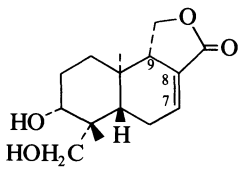
[66924-15-0]



$CHIN_4$ M 195.950
Cryst. (EtOH). Sol. hot H_2O, spar. sol. Et_2O. Mp 190°. pK_a 4.66.
1-Ph:
$C_7H_5IN_4$ M 272.048
Cryst. (EtOH). Mp 140° dec.
Stollé, R. *et al*, *Ber.*, 1929, **62**, 1118 (*synth*)
Stollé, R. *et al*, *J. Prakt. Chem.*, 1932, **134**, 282 (*deriv*)
Leiber, E. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 1792 (*props*)

Iresin I-80043

Updated Entry replacing I-00832



$C_{15}H_{22}O_4$ M 266.336
Constit. of *Iresine celosioides*. Cryst. (Me_2CO/hexane). Mp 140-142°. $[\alpha]_D^{28}$ +21° ($CHCl_3$).

7,8β-Dihydro: ***Dihydroiresin***
$C_{15}H_{24}O_4$ M 268.352
Minor constit. of *I. celosioides*. Mp 212-213° (as diacetate).

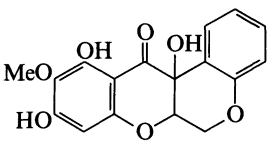
$\Delta^{8,9}$*-Isomer:* [561-89-7]. ***Isoiresin***
$C_{15}H_{22}O_4$ M 266.336
Constit. of *I. celosioides*. Oil. Mp 166-168° (as diacetate). $[\alpha]_D$ −73.0° ($CHCl_3$) (diacetate).

7,8β-Dihydro, 3-ketone: ***Dihydroiresone***
$C_{15}H_{22}O_4$ M 266.336
Isol. from *I. celosioides*. Needles (C_6H_6/MeOH). Mp 215-219°.

Crabbé, P. *et al*, *Bull. Soc. Chim. Belg.*, 1958, **67**, 632 (*derivs*)
Djerassi, C. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 2593 (*struct*)
Rossmann, H.G. *et al*, *Tetrahedron*, 1958, **4**, 275 (*cryst struct*)
Pettetier, S.W. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5318 (*synth*)

Irispurinol I-80044

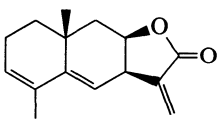
[119459-73-3]



$C_{17}H_{14}O_7$ M 330.293
Constit. of *Iris spuria*. Pale yellow needles (EtOAc). Mp 255-256°. $[\alpha]_D^{22}$ −75.2° (MeOH).

Shawl, A.S. *et al*, *Phytochemistry*, 1988, **27**, 3331.

Isoalantodiene I-80045

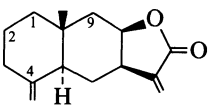


$C_{15}H_{18}O_2$ M 230.306
Constit. of *Inula racemosa*. Cryst. Mp 82°.

Kalsi, P.S. *et al*, *Phytochemistry*, 1989, **28**, 2093 (*isol, pmr*)

Isoalantolactone I-80046

Updated Entry replacing I-30064
Isohelenin
[470-17-7]



$C_{15}H_{20}O_2$ M 232.322
Constit. of the essential oil of *Inula helenium*, *I. racemosa* and *Telekia speciosa*. Cryst. (EtOH aq.). Mp 109-110° (115°). $[\alpha]_D$ +172° ($CHCl_3$).

1α,2α-Diacetoxy: ***1α,2α-Diacetoxyalantolactone***
$C_{19}H_{24}O_6$ M 348.395
Constit. of *Inezia integrifolia*. Gum. $[\alpha]_D^{24}$ +68° (c, 0.11 in $CHCl_3$).

1-Oxo: ***1-Oxoisoalantolactone***
$C_{15}H_{18}O_3$ M 246.305
Constit. of *Flourensia macrophylla*. Cryst. Mp 164°. Incorrectly called 1-Oxoalantolactone in the lit.

!9α-Hydroxy: 9α-Hydroxyisoalantolactone
$C_{15}H_{20}O_3$ M 248.321
Constit. of *F. macrophylla*. Oil. Incorrectly called 9-Hydroxyalantolactone.

9β-Hydroxy: ***9β-Hydroxyisoalantolactone***
$C_{15}H_{20}O_3$ M 248.321
Isol. from *F. macrophylla*. Cryst. Mp 171°. $[\alpha]_D^{24}$ +78° (c, 1.9 in $CHCl_3$).

9-Oxo: ***9-Oxoisoalantolactone***
$C_{15}H_{18}O_3$ M 246.305
Isol. from *F. macrophylla*. Cryst. Mp 118°. Incorrectly called 9-Oxoalantolactone.

4α,15-Epoxy: ***4α,15-Epoxyisoalantolactone***
$C_{15}H_{20}O_3$ M 248.321
Constit. of *Ambrosia artemisioides*. Oil.

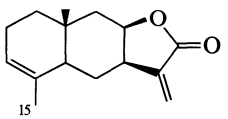
4α,15-Epoxy, 3α-hydroxy: ***4α,15-Epoxy-3α-hydroxyisoalantolactone***
$C_{15}H_{20}O_4$ M 264.321
Constit. of *A. artemisioides*. Oil.

11,12-Dihydro: ***Dihydroisoalantolactone***
$C_{15}H_{22}O_2$ M 234.338
Isol. from roots of *I. helenium*. Needles (EtOH). Mp 168-174°.

Asselineau, C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1958, **246**, 1874 (*struct*)
Marshall, J.A. *et al*, *J. Org. Chem.*, 1964, **29**, 3727 (*pmr, struct*)
Miller, R.B. *et al*, *Tetrahedron*, 1974, **30**, 2961 (*synth*)
Tada, M., *Chem. Lett.*, 1982, 441 (*synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1982, **21**, 2743 (*derivs*)
Bohlmann, F. *et al*, *Phytochemistry*, 1984, **23**, 1445 (*derivs*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551 (*derivs*)

Isoalloalantolactone I-80047

Updated Entry replacing I-40044
[64395-76-2]



$C_{15}H_{20}O_2$ M 232.322
Constit. of *Inula racemosa*. Oil.

15-Hydroxy: [119285-33-5]. ***15-Hydroxyisoalloalantolactone***
$C_{15}H_{20}O_3$ M 248.321
Constit. of *Ambrosia artemisioides*. Oil.

15-Acetoxy: [119285-34-6]. ***15-Acetoxyisoalloalantolactone***
$C_{17}H_{22}O_4$ M 290.358
Constit. of *A. artemisioides*. Oil.

15-Cinnamoyloxy (E-): [119285-35-7]. ***15-Cinnamoyloxyisoalloalantolactone***
$C_{24}H_{26}O_4$ M 378.467
Constit. of *A. artemisioides*. Oil.

15-Cinnamoyloxy (Z-): [119285-36-8].
$C_{24}H_{26}O_4$ M 378.467

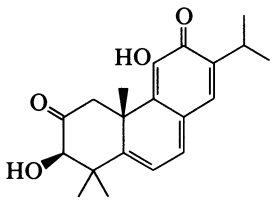
Constit. of *A. artemisioides*. Oil.

Kaur, B. *et al*, *Phytochemistry*, 1985, **24**, 2007 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551 (*derivs*)

Isobharangin I-80048

3β,11-Dihydroxy-5,7,9,13-abietatetraene-2,12-dione

[121688-14-0]



$C_{20}H_{24}O_4$ M 328.407

Constit. of *Pygmacopremna herbacea*. Brown solid. Mp 74-76°. $[\alpha]_D^{26}$ −465° (c, 0.115 in $CHCl_3$).

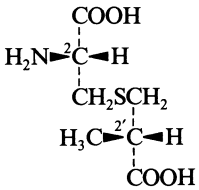
Sankaram, A.V.B. *et al*, *Tetrahedron Lett.*, 1989, **30**, 867.

Isobuteine I-80049

Updated Entry replacing I-30069

S-(*2-Carboxypropyl*)*cysteine*, *9CI*. *3-*[(*2-Carboxypropyl*)*thio*]*alanine*

[4746-40-1]



(*2R,2'S*)-*form*

$C_7H_{13}NO_4S$ M 207.250

(***2R,2'S***)-***form*** [66512-75-2]

Occurs naturally as a component of the tripeptide *S*-(2-carboxypropyl)glutathione in onion and in garlic. Also isol. from urine of cystathionuric patients. Intermed. in biosynth. of cycloalliin. Cryst. (Me_2CO aq.). Mp 196-198° dec. $[\alpha]_D^{25}$ −66.1° (c, 2.5 in H_2O), −44.3° (c, 2.4 in2.5M HCl). Diastereoisomers also known.

S,S-*Dioxide:* [66403-99-4]. *3-*[(*2-Carboxypropyl*)*sulfonyl*]*alanine*, *9CI*

$C_7H_{13}NO_6S$ M 239.249

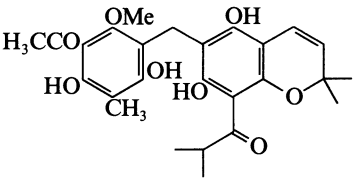
Blades (H_2O). Mp 174° dec. (gas evolution). $[\alpha]_D^{25}$ −24° (c, 1.7 in H_2O).

[6852-42-2, 66429-71-8, 66512-76-3]

Virtanen, A.I. *et al*, *Hoppe Seyler's Z. Physiol. Chem.*, 1960, **322**, 8 (*isol*)
Granroth, B. *et al*, *Acta Chem. Scand.*, 1967, **21**, 1654 (*bisynth*)
Carson, J.F., *J. Chem. Soc., Perkin Trans.* 1, 1977, 1964 (*synth, pmr*)
Kasai, T. *et al*, *Agric. Biol. Chem.*, 1981, **45**, 433 (*occur*)
Parry, R.J. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 2512 (*synth, abs config*)

Isobutyrylmallotochromene I-80050

[116964-16-0]

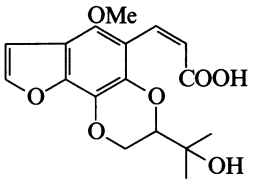


$C_{26}H_{30}O_8$ M 470.518

Constit. of *Mallotus japonicus*. Cytotoxic agent. Yellow needles (MeOH). Mp 180-181°.

Fujita, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 708.

Isobyakangelicolic acid I-80051

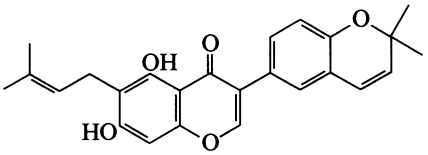


$C_{17}H_{18}O_7$ M 334.325

Doubtful struct. Isol. from *Angelica japonica* and *A. glabra*. Tablets (EtOH). Mp 220°. $[\alpha]_D^{16}$ +5.3° (Py).

Noguchi, T. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1941, **61**, 77 (*isol*)
Hata, K. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1960, **54**, 25581 (*isol*)

Isochandalone I-80052



$C_{25}H_{24}O_5$ M 404.462

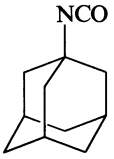
Constit. of *Lupinus albus*. Amorph. powder.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

1-Isocyanatoadamantane I-80053

1-Isocyanatotricyclo[*3.3.1.1*^{3,7}]*decane*, *9CI*. *1-Adamantyl isocyanate*

[4411-25-0]



$C_{11}H_{15}NO$ M 177.246

Cryst. Mp 147°.

Stetter, H. *et al*, *Chem. Ber.*, 1962, **95**, 2302 (*synth*)
Boyer, J.H. *et al*, *Synthesis*, 1987, 907 (*synth*)

Isocyanatodiphenylmethane I-80054

1,1'-(*Isocyanatomethylene*)*bisbenzene*, *9CI*. *Diphenylmethyl isocyanate*

[3066-44-2]

Ph_2CHNCO

$C_{14}H_{11}NO$ M 209.247
Liq. Bp_4 148°.

Donleavy, J.J. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 218 (*synth*)
Boyer, J.H. *et al*, *Synthesis*, 1987, 907 (*synth*)

(Isocyanatomethyl)benzene, 9CI — I-80055

Benzyl isocyanate
[3173-56-6]

$PhCH_2NCO$

C_8H_7NO M 133.149
Liq. Bp_{30} 137°, Bp_4 65°.

Ferstandig, L.L. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 4838 (*synth*)
Boyer, J.H. *et al*, *Synthesis*, 1987, 907 (*synth*)

Isocyanatotriphenylmethane — I-80056

1,1′,1″-(Isocyanatomethylidyne)trisbenzene, 9CI. Triphenylmethyl isocyanate. Trityl isocyanate
[4737-21-7]

Ph_3CNCO

$C_{20}H_{15}NO$ M 285.345
Cryst. (pet. ether). V. sol. org. solvs. Mp 91° (85-87°).

Jones, L.W. *et al*, *J. Am. Chem. Soc.*, 1921, **43**, 2422 (*synth*)
Boyer, J.H. *et al*, *Synthesis*, 1987, 907 (*synth*)

Isocyanic acid, 8CI — I-80057

Updated Entry replacing I-20052
[75-13-8]

HN=C=O

CHNO M 43.025
Contrary to popular belief, is not in equilib. with Cyanic acid, C-80167. Is freq. confused with cyanic acid in CA. Reagent for conversion of alcohols to allophanates. Also adds to carbonyl compds. and alkenes. Liq. or gas with strongly acrid odour. d^0 1.140. Mp −86°. Bp 23.5°. pK_a 3.66. For esters (isocyanates) see the individual entries.

▷ Lachrymator, vesicant.

v. Dohlen, W.C. *et al*, *Acta Crystallogr.*, 1955, **8**, 646 (*struct, synth, ir*)
Steyemark, P.R., *J. Org. Chem.*, 1963, **28**, 586 (*synth*)
Groving, N. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1768 (*synth*)
Belson, D.J. *et al*, *Chem. Soc. Rev.*, 1982, **11**, 41 (*rev*)
Teles, J.H. *et al*, *Chem. Ber.*, 1989, **122**, 753 (*struct, bibl*)

1-Isocyanobutane, 9CI — I-80058

Butyl isocyanide
[2769-64-4]

$H_3CCH_2CH_2CH_2NC$

C_5H_9N M 83.133
Extremely disagreeable and pervasive smelling liq. d 0.80. Bp 124-125°.

▷ Causes headaches and nausea.

Davis, T.L. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 1998 (*synth*)
Malatesta, L., *Gazz. Chim. Ital.*, 1947, **77**, 238 (*synth*)
Ugi, I. *et al*, *Chem. Ber.*, 1960, **93**, 239 (*synth, ir*)
Kamer, P.C.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6818 (*synth, ir, pmr*)

3-Isocyanopentane, 9CI — I-80059

3-Pentyl isocyanide
[115591-41-8]

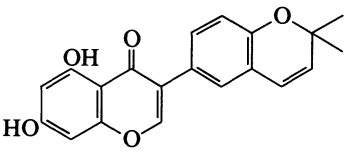
$(H_3CCH_2)_2CHNC$

$C_6H_{11}N$ M 97.160

Kamer, P.C.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6818 (*synth, ir, pmr*)

Isoderrone — I-80060

[121747-89-5]

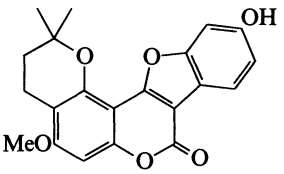


$C_{20}H_{16}O_5$ M 336.343
Constit. of *Lupinus albus*. Amorph. solid.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Isoglycyrol — I-80061

3,4-Dihydro-11-hydroxy-5-methoxy-2,2-dimethyl-2H,8H-benzofuro[3,2-c]pyrano[2,3-f][1]benzopyran-8-one, 9CI
[23013-86-7]



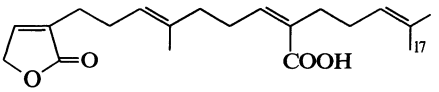
$C_{21}H_{18}O_6$ M 366.370
Isol. from roots of *Glycyrrhiza* sp. Needles (Me_2CO). Mp 298-300° dec.

Ac: Needles (MeOH). Mp 175-176°, Mp 197-197.5° (double Mp).

Me ether: Pale-yellow needles (Me_2CO). Mp 225.5-224°.

Saitoh, T. *et al*, *Chem. Pharm. Bull.*, 1969, **17**, 729.

Isogutiesolbriolide — I-80062



$C_{20}H_{28}O_4$ M 332.439
Parent compd. unknown. L540.

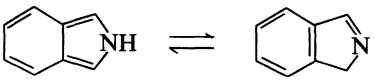
17-Hydroxy: ***17-Hydroxyisogutiesolbriolide***
$C_{20}H_{28}O_5$ M 348.438
Constit. of *Gutierrezia solbrigii*.

17-Acetoxy: ***17-Acetoxyisogutiesolbriolide***
$C_{22}H_{30}O_6$ M 390.475
Constit. of *G. solbrigii*.

Jakupovic, J. *et al*, *Tetrahedron*, 1985, **41**, 4537.

Isoindole — I-80063

Updated Entry replacing I-20061
Benzo[c]pyrrole
[270-68-8]



C_8H_7N M 117.150
Solid obt. by pyrolysis and freezing at −196°. λ_{max} 263.5, 275, 286.5, 294 (infl.), 300, 306.5, 312.5, 320, 326.5 and 335 nm(hexane).Solid dec. rapidly at r.t., mod. stable in soln. under N_2.

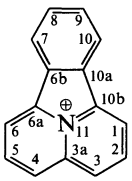
N-tert-*Butyl:* [55023-87-5].
$C_{12}H_{15}N$ M 173.257
Bp_{11} 97-98°.

N-tert-*Butyl; B,HClO$_4$:* [73286-77-8].
Cryst. Mp 241-243° dec.

Kreher, R. *et al*, *Z. Naturforsch.*, *B*, 1965, **20**, 75 (*synth*)
White, J.D. *et al*, *Adv. Heterocycl. Chem.*, 1969, **10**, 113 (*rev*)
Dewar, M.J.S. *et al*, *Tetrahedron*, 1970, **26**, 4505 (*props*)
Bonnett, R. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1973, 1432 (*synth*)
Chacko, E. *et al*, *Tetrahedron Lett.*, 1977, 1095 (*props*)
Bonnett, R. *et al*, *Adv. Heterocycl. Chem.*, 1981, **29**, 341 (*rev*)
Kreher, R.P. *et al*, *Chem. Ber.*, 1989, **122**, 337 (*derivs*)

Isoindolo[1,2,3-*de*]quinolizinium(1+), 9CI I-80064

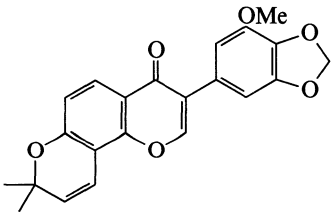
10c-Azoniafluoranthene



$C_{15}H_{10}N^{\oplus}$ M 204.251 (ion)
Hexafluorophosphate: [120229-35-8].
$C_{15}H_{10}F_6NP$ M 349.215
Transparent needles (MeCN).

Fourmigué, M. *et al*, *Angew. Chem.*, *Int. Ed. Engl.*, 1989, **28**, 588 (*synth*, *pmr*, *struct*, *cmr*, *uv*)

Isojamaicin I-80065

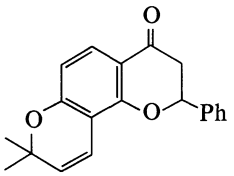


$C_{22}H_{18}O_6$ M 378.381
Constit. of *Millettia ferruginea*. Amorph.

Dagne, E. *et al*, *Phytochemistry*, 1989, **28**, 1897.

Isolonchocarpin I-80066

Updated Entry replacing I-01090
*2,3-Dihydro-8,8-dimethyl-2-phenyl-4*H,*8*H-*benzo*[*1,2*-b:*3,4*-b′]*dipyran-4-one*



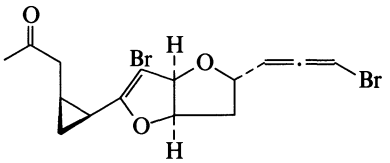
$C_{20}H_{18}O_3$ M 306.360
(−)-***form*** [34198-88-4]
Constit. of the seed oil of *Pongamia glabra* and of the roots of *Tephrosia purpurea* and *Derris sericea*. Needles (hexane). Mp 115°. $[\alpha]_D^{24}$ −125° ($CHCl_3$).

4′-Hydroxy: ***4′-Hydroxyisolonchocarpin***
$C_{20}H_{18}O_4$ M 322.360
Constit. of *Millettia ferruginea*. Amorph.

Satam, P.G.N. *et al*, *Indian J. Chem.*, 1973, **11**, 209 (*isol*, *struct*)
Subrahmanyam, K. *et al*, *Indian J. Chem.*, *Sect. B*, 1977, **15**, 105 (*synth*)
Jain, A.C. *et al*, *Proc.-Indian Acad. Sci.*, *Sect. A*, 1978, **87**, 247 (*synth*)
Rao, E.V. *et al*, *Phytochemistry*, 1979, **18**, 1581 (*isol*)
Dagne, E. *et al*, *Phytochemistry*, 1989, **28**, 1897 (*deriv*)

Isookamurallene I-80067

Updated Entry replacing I-10105

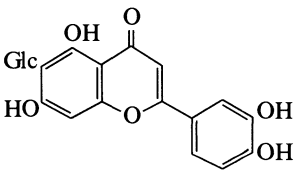


$C_{15}H_{16}Br_2O_3$ M 404.098
Oil. $[\alpha]_D^{27}$ +130° (c, 1.00 in $CHCl_3$).

Suzuki, M. *et al*, *Chem. Lett.*, 1982, 289 (*isol*)
Suzuki, M. *et al*, *Phytochemistry*, 1989, **28**, 2145 (*struct*)

Isoorientin I-80068

Updated Entry replacing I-10106
*2-(3,4-Dihydroxyphenyl)-6-β-D-glucopyranosyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one*, *9CI. 6-*C*-Glucopyranosyl-3′,4′,5,7-tetrahydroxyflavone. 6-*C*-β-D-Glucopyranosylluteolin. Homoorientin. Lespecapitoside. Lutonaretin*
[4261-42-1]



$C_{21}H_{20}O_{11}$ M 448.382
Widespread occurrence in *Adonis*, *Gentiana*, *Helenium* and *Passiflora* spp., etc. Light-yellow needles. Mp 235°. $[\alpha]_D^{20}$ +30.8° (c, 1.2 in Py).

4′-Glucoside:
$C_{27}H_{30}O_{16}$ M 610.524
Constit. of the leaves of *G. verna*. Cryst. (H_2O). Mp 216° dec.

7-Glucoside: [35450-86-3]. ***Lutonarin***
$C_{27}H_{30}O_{16}$ M 610.524
Found in barley (*Hordeum vulgare*) and other plants in Graminae, Leguminosae and Lemnaceae. Bright yellow cryst. Mp 235° dec.

2″-(4-Hydroxybenzoyl), 4′-β-D-glucopyranoside:
$C_{34}H_{34}O_{18}$ M 730.632
Constit. of *Gentiana asclepiadea*. Cryst. (MeOH). Mp 204-205°.

*2″-*O*-Glucosyl: 3′,4′,5,7-Tetrahydroxy-*6*-*C*-sophorosylflavone*
$C_{27}H_{30}O_{16}$ M 610.524
Constit. of the leaves of *G. verna*. Cryst. (MeOH). Mp 212°.

2″,4′-Diglucosyl:
$C_{33}H_{40}O_{21}$ M 772.666

Constit. of the leaves of *G. asclepiadea*. Mp 211-213° dec.

3-Me ether, 7-O-β-D-glucopyranoside: 3′-O-Methyllutonarin
$C_{28}H_{32}O_{16}$ M 624.551
Isol. from leaves of *Hordeum vulgare*. Amorph. light-yellow powder. Mp 190-195° dec. Struct. revision resulting from revised struct. of Isoorientin.

2″-(4-Hydroxybenzoyl):
$C_{28}H_{24}O_{13}$ M 568.490
Constit. of *Gentiana asclepiadea*.

Seikel, M.K. *et al*, *Arch. Biochem. Biophys.*, 1962, **99**, 451 (3′-O-Methylutonarin)
Koeppen, B.H. *et al*, *Biochem. J.*, 1965, **97**, 444 (*struct*)
Chopin, J. *et al*, *Tetrahedron Lett.*, 1966, 3657 (*synth*)
Hostettmann, K. *et al*, *Helv. Chim. Acta*, 1975, **58**, 130 (2″-*Glucosyl*)
Goetz, M. *et al*, *Helv. Chim. Acta*, 1977, **60**, 1322; 1978, **61**, 1373 (*deriv*)
Hostettmann, M. *et al*, *Phytochemistry*, 1978, **17**, 2083 (*rev*)
Congora, C. *et al*, *Helv. Chim. Acta*, 1986, **69**, 251 (*isol*)

8(14),15-Isopimaradiene-3,18-diol I-80069

8,(14),15-Sandaracopimaradiene-3,18-diol
$C_{20}H_{32}O_2$ M 304.472

3β-form
Isol. from wood of *Xylia dolabriformis*. Platelets (pet. ether). Mp 152-153°. $[\alpha]_D$ −18.5° (c, 4 in $CHCl_3$).

Laidlaw, R.A. *et al*, *J. Chem. Soc.*, 1963, 644.

8(14),15-Isopimaradiene-2,3,18,19-tetrol I-80070

8(14),15-Sandaracopimaradiene-2,3,18,19-tetrol
$C_{20}H_{32}O_4$ M 336.470

(2α,3β)-form
***Dacrydol* D_1**
Isol. from *Dacrydium colensoi*. Mp 210-240°.

Carman, R.H. *et al*, *Tetrahedron Lett.*, 1966, 3173.

8(14),15-Isopimaradiene-2,18,19-triol I-80071

8(14),15-Sandaracopimaradiene-2,18,19-triol
$C_{20}H_{32}O_3$ M 320.471

2α-form
***Dacrydol* D_2**
Isol. from *Dacrydium colensoi*. Mp 224-227°.

Carman, R.N. *et al*, *Tetrahedron Lett.*, 1966, 3173.

8(14),15-Isopimaradiene-3,18,19-triol I-80072

8(14),15-Sandaracopimaradiene-3,18,19-triol
$C_{20}H_{32}O_3$ M 320.471

3β-form
***Dacrydol* D_3**
Isol. from *Dacrydium colensoi*. Mp 163-166°.

Carman, R.M. *et al*, *Tetrahedron Lett.*, 1966, 3173.

8,15-Isopimaradien-18-oic acid I-80073

$\Delta^{8(9)}$-Isopimaric acid
$C_{20}H_{30}O_2$ M 302.456
Found in resin of *Pinus* spp. esp. *P. edulis*; also in *Tetraclinis* spp., *Callitris* spp. and *Dacrydium biforme*. Cryst. Mp 105-106°. $[\alpha]_D$ +94° (c, 1.14 in $CHCl_3$).

Me ester: Cryst. (MeOH). Mp 68-70°. $[\alpha]_D$ +118° (c, 1.0 in EtOH).

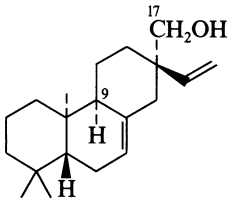
Edwards, O.E. *et al*, *Can. J. Chem.*, 1959, **37**, 760 (*synth*)
ApSimon, J.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 361 (*pmr*)
Joye, N.M. *et al*, *J. Org. Chem.*, 1966, **31**, 320 (*occur*)

8(14),15-Isopimaradien-18-ol I-80074

8(14),15-Sandaracopimaradien-18-ol. ***Sandaracopimarinol***
$C_{20}H_{32}O$ M 288.472
Isol. from *Cryptomeria japonica* and *Agathis australis*. Cryst. Mp 63-65°. $[\alpha]_D$ −11° (c, 2.34 in $CHCl_3$).

Nagahama, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1964, **37**, 886.
Thomas, B.R., *Acta Chem. Scand.*, 1966, **20**, 1074.

ent-9β*H*-Isopimara-7,15-dien-17-ol I-80075



$C_{20}H_{32}O$ M 288.472
Constit. of *Calceolaria foliosa*. Cryst. Mp 75-76°. $[\alpha]_D^{25}$ −160.6° (c, 1 in $CHCl_3$).

Ac: ent-17-*Acetoxy*-9β*H*-*isopimara*-7,15-*diene*
$C_{22}H_{34}O_2$ M 330.509
Constit. of *C. foliosa*. Oil. $[\alpha]_D^{25}$ −120.6° (c, 1.02 in $CHCl_3$).

Malonyl: ent-17-*Malonyloxy*-9β*H*-*isopimara*-7,15-*diene*
$C_{23}H_{34}O_4$ M 374.519
Constit. of *C. foliosa*. Oil. $[\alpha]_D^{25}$ −127.5° (c, 1 in $CHCl_3$).

17-Carboxylic acid: **ent-9βH-*Isopimara-7,15-dien-17-oic acid***
$C_{20}H_{30}O_2$ M 302.456
Constit. of *C. foliosa*. Cryst. Mp 160-161°. $[\alpha]_D^{25}$ −174.2° (c, 1 in $CHCl_3$).

Chamy, M.C. *et al*, *Phytochemistry*, 1989, **28**, 571.

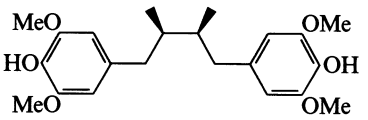
8(14),15-Isopimaradien-3-one I-80076

8(14),15-Sandaracopimaradien-3-one
$C_{20}H_{30}O$ M 286.456
Isol. from heartwood of *Xylia dolabriformis*. Platelets (MeOH). Mp 59-60°. $[\alpha]_D$ −56° (c, 2 in $CHCl_3$).

Laidlaw, R.A. *et al*, *J. Chem. Soc.*, 1963, 644 (*isol, ir, struct*)
Grant, P.K. *et al*, *Tetrahedron Lett.*, 1965, 3729 (*synth*)

Isopregomisin I-80077

[122222-00-8]



$C_{22}H_{30}O_6$ M 390.475
Constit. of *Porlieria chilensis*. Cryst. Mp 110-112°. *meso*.

Torres, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 402 (*isol, pmr, cmr*)

4-Isopropylbenzyl alcohol I-80078

Updated Entry replacing I-01224
4-(1-Methylethyl)benzenemethanol, 9CI. p-*Cymen-7-ol, 8CI. Cuminyl alcohol. Cumic alcohol*

[536-60-7]

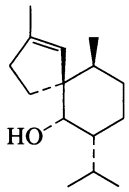
$C_{10}H_{14}O$ M 150.220
Bp 246°, Bp_{20} 140°.

▷ GZ7260000.
Ac: [59230-57-8].
$C_{12}H_{16}O_2$ M 192.257
$Bp_{16.5}$ 136°.
O-[*β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside*]: ***Coleoside***
$C_{22}H_{34}O_{11}$ M 474.504
Constit. of *Coleus forskohlii*. Yellow solid.

Bert, L., *Bull. Soc. Chim. Fr.*, 1925, **37**, 1397, 1577 (*synth*)
Palfray, L. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1936, **203**, 1523 (*synth*)
v. Tamelen, E.E. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 5290 (*synth*)
Ahmed, B. *et al*, *Phytochemistry*, 1988, **27**, 3309 (*Coleoside*)

7-Isopropyl-2,10-dimethylspiro[4.5]dec-1-en-6-ol I-80079

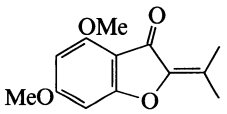
2,10-Dimethyl-7-(1-methylethyl)spiro[4.5]dec-1-en-6-ol, 9CI
[119432-99-4]



$C_{15}H_{26}O$ M 222.370
Constit. of a *Eurypon* sp. Oil. $[\alpha]_D$ +1.3° (c, 0.6 in $CHCl_3$). Related to Axisisonitrile 3

Barrow, C.J. *et al*, *Aust. J. Chem.*, 1988, **41**, 1755.

2-Isopropylidene-4,6-dimethoxy-3(2*H*)-benzofuranone I-80080

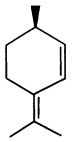


$C_{13}H_{14}O_4$ M 234.251
Constit. of *Calea peckii*. Oil.

Castro, V. *et al*, *Phytochemistry*, 1989, **28**, 2415 (*isol, pmr*)

3-Isopropylidene-6-methylcyclohexene I-80081

Updated Entry replacing I-01304
2,4(8)-p-*Menthadiene*. ***Menogene***
[586-63-0]

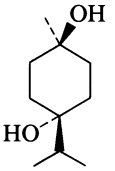


$C_{10}H_{16}$ M 136.236
(R)-form
Isol. from leaf oil of *Juniperus horizontalis*. Oil. $Bp_{764.5}$ 184-186°. $[\alpha]_D^{17}$ +49.1°. n_D^{20} 1.5026.

Ohloff, G. *et al*, *Justus Liebigs Ann. Chem.*, 1959, **625**, 206 (*synth, uv, abs config*)
Couchman, F.M. *et al*, *Can. J. Chem.*, 1965, **43**, 1017 (*isol*)
Verghese, J., *Perfum. Essent. Oil Rec.*, 1967, **58**, 868 (*rev*)
Bark, S. *et al*, *J. Org. Chem.*, 1968, **33**, 221 (*synth*)
Bohlmann, F. *et al*, *Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)

1-Isopropyl-4-methyl-1,4-cyclohexanediol I-80082

p-*Menthane-1,4-diol*

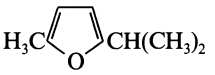


$C_{10}H_{20}O_2$ M 172.267
(1RS,4RS)-form
(1*β*,4*α*)-*form*
Constit. of *Ferula jaeshkeana*. Cryst. Mp 153°.

Garg, S.N. *et al*, *Phytochemistry*, 1989, **28**, 634.

2-Isopropyl-5-methylfuran I-80083

2-Methyl-5-(1-methylethyl)furan
[10504-05-9]

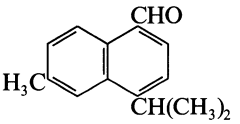


$C_8H_{12}O$ M 124.182
Important natural flavour. Oil with strong herbaceous odour. Bp 136°, Bp_{60} 58°.

Heyns, K. *et al*, *Tetrahedron*, 1966, **22**, 2223 (*ms*)
Eichenberger, H. *et al*, *Helv. Chim. Acta*, 1976, **59**, 1253 (*cmr*)
Weyerstahl, P. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 1015 (*synth, pmr, bibl*)

4-Isopropyl-7-methyl-1-naphthalenecarboxaldehyde I-80084

7-Methyl-4-(1-methylethyl)-1-naphthalenecarboxaldehyde. 14-Cadalenal



$C_{15}H_{16}O$ M 212.291
Constit. of *Helichrysum ambiguum*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 543.

Isopropyl phenyl ether I-80085

(1-Methylethoxy)benzene, 9CI. 2-Phenoxypropane. Isopropoxybenzene
[2741-16-4]

$PhOCH(CH_3)_2$

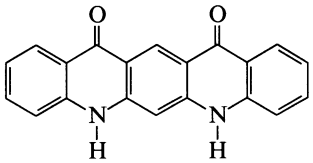
$C_9H_{12}O$ M 136.193
d^{20} 0.978. Fp −33.05°. Bp 178°. n_D^{20} 1.4975.

Sadtler Standard Infrared Spectra, No. 11619 (*ir*)
Smith, R.A., *J. Am. Chem. Soc.*, 1934, **56**, 717 (*synth*)
Olson, W.T. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 2451 (*synth*)
Vogel, A.I., *J. Chem. Soc.*, 1948, 616 (*props*)
Baddeley, G. *et al*, *J. Chem. Soc.*, 1956, 2455 (*uv*)

Isoquinacridone I-80086

*Quino-[3,2-*b*]acridine-12,14(*5H,7H*)-dione, 9CI. 5,7-Dihydroquino[3,2-*b*]acridine-12,14-dione.* lin-cis-*Quinacridone*

[3164-44-1]



$C_{20}H_{12}N_2O_2$ M 312.327

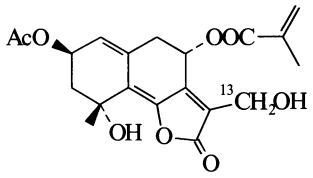
Brownish-yellow needles ($PhNO_2$). Prac. insol. most solvs.

Eckert, A. *et al*, *J. Prakt. Chem.*, 1921, **102**, 338 (*synth*)
Leandri, G. *et al*, *Boll. Sci. Fac. Chim. Ind. Bologna*, 1951, **9**, 32; *CA*, **45**, 10245e (*synth, props*)
Labana, S.S. *et al*, *Chem. Rev.*, 1967, **67**, 1 (*rev*)
Altiparmakian, R.H. *et al*, *Helv. Chim. Acta*, 1972, **55**, 85 (*pmr*)

Isorolandrolide I-80087

Updated Entry replacing I-01549

[76010-19-0]



$C_{21}H_{26}O_8$ M 406.432

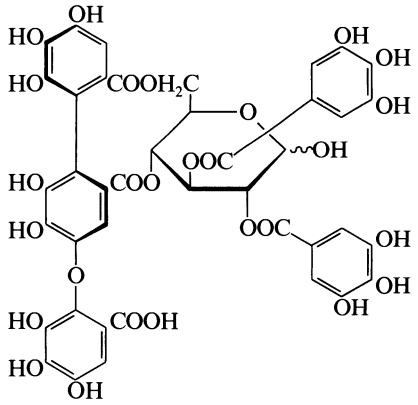
Constit. of *Rolandra fruticosa*. Gum.

13-Et ether: [76010-18-9].
$C_{23}H_{30}O_8$ M 434.485
Constit. of *R. fruticosa*. Noncryst.

Herz, W. *et al*, *J. Org. Chem.*, 1981, **46**, 761 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1937 (*struct*)

Isorugosin B I-80088

[119139-61-6]



$C_{41}H_{30}O_{27}$ M 954.672

Constit. of *Liquidamber formosa*. Light brown amorph. powder. $[\alpha]_D$ +28° (c, 1 in MeOH).

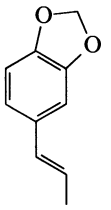
Hatano, T. *et al*, *Heterocycles*, 1988, **27**, 2081.

Isosafrole I-80089

Updated Entry replacing M-30101

5-(1-Propenyl)-1,3-benzodioxole, 9CI. 1,2-(Methylenedioxy)-4-(1-propenyl)benzene, 8CI

[120-58-1]



(*E*)-*form*

$C_{10}H_{10}O_2$ M 162.188

Isol. from star anise oil (*Illicium religiosum*), seed oil of *Ligusticum acutilobum* and leaves of *Murraya koenigi*.

(E)-form [4043-71-4]

β-Isosafrole

Perfumery intermed. Fp 6.7-6.8°. Bp_{768} 252.4-252.7°, $Bp_{11.5}$ 123°.

▷ DA5951000.

(Z)-form [17627-76-8]

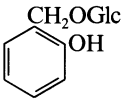
α-Isosafrole

Present in essential oils. Liq.

Crymble, C.R. *et al*, *J. Chem. Soc.*, 1911, 451 (*uv*)
Robinson, R. *et al*, *J. Chem. Soc.*, 1927, 2489 (*synth*)
Dutt, S., *CA*, 1958, **52**, 20904 (*isol*)
Willhalm, B. *et al*, *Tetrahedron*, 1964, **20**, 1185 (*ms*)
Shulgin, A.T., *J. Chromatogr.*, 1967, **30**, 54 (*glc*)
Torii, S. *et al*, *J. Org. Chem.*, 1984, **49**, 1830 (*synth*)

Isosalicin I-80090

[7724-09-6]



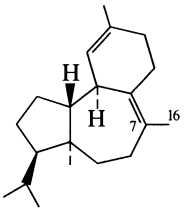
$C_{13}H_{18}O_7$ M 286.281

Isol. from flowers of *Filipendula ulmaria*. Needles + $3H_2O$ (Me_2CO/pet. ether). Mp 66-68°. $[\alpha]_D^{20}$ −45.2° (anhyd.).

Bourquelot, E. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1913, **156**, 1790 (*synth*)
Thieme, H., *Pharmazie*, 1966, **21**, 123 (*isol*)

Isosphaerodiene 1 I-80091

[80981-70-0]



$C_{20}H_{32}$ M 272.473

Constit. of *Sphaerococcus coronopifolius*. Oil. $[\alpha]_D$ +28° ($CHCl_3$).

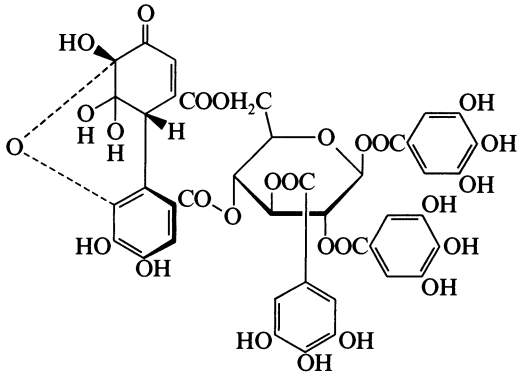
$\Delta^{7(16)}$-*Isomer:* [108907-24-0]. ***Isosphaerodiene 2***
$C_{20}H_{32}$ M 272.473
Constit. of *S. coronopifolius*. Oil. $[\alpha]_D$ +18° ($CHCl_3$).

Cafieri, F. *et al*, *Phytochemistry*, 1987, **26**, 471.

Isoterchebin I-80092

1,2,3-Tri-O-galloyl-4,6-O-dehydrohexahydroxydiphenoyl-β-D-glucopyranose. Cornus-tannin 1

[58690-20-3]



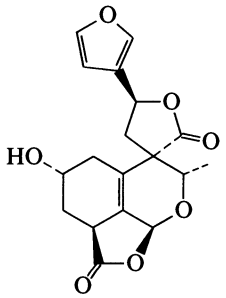
$C_{41}H_{30}O_{26}$ M 938.672

Isol. from *Cytinus hypocistis* and *Cornus officinalis*. Hygroscopic solid + $6H_2O$.

Fürstenwerth, H. *et al*, *Justus Liebigs Ann. Chem.*, 1976, 112 (*isol, pmr*)

Okuda, T. *et al*, *Heterocycles*, 1981, **16**, 1321 (*struct*)

Isoteucrin H_4 I-80093



$C_{19}H_{20}O_6$ M 344.363

Constit. of *Teucrium kotschyanum*.

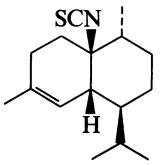
Ac: Cryst. (EtOAc/hexane). Mp 191-194°. $[\alpha]_D^{22}$ +128.6° (c, 0.168 in $CHCl_3$).

Simões, F. *et al*, *Heterocycles*, 1989, **28**, 111.

1-Isothiocyanato-4-cadinene I-80094

4-Cadinene-1-isothiocyanate

[117605-65-9]

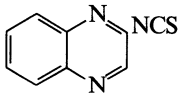


$C_{16}H_{25}NS$ M 263.446

Metab. of the sponge *Acanthella pulcherrima*.

Capon, R.J. *et al*, *Aust. J. Chem.*, 1988, **41**, 979.

2-Isothiocyanatoquinoxaline I-80095



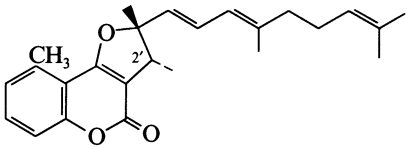
$C_9H_5N_3S$ M 187.225

Pale yellow needles (pet. ether). Mp 48-48.5°.

Ijima, C. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1988, **108**, 437.

Isotriptiliocoumarin I-80096

[118627-71-7]



$C_{25}H_{30}O_3$ M 378.510

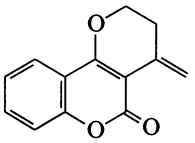
Constit. of *Triptilion benaventei*. Gum.

2'-Epimer: [118555-94-5]. ***2'-Epiisotriptiliocoumarin***
$C_{25}H_{30}O_3$ M 378.510
Constit. of *T. benaventei*. Gum.

Bittner, M. *et al*, *Phytochemistry*, 1988, **27**, 3263.

Isotriptospinocoumarin I-80097

[119875-30-8]



$C_{14}H_{12}O_3$ M 228.247

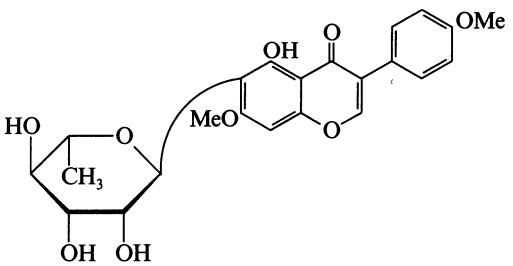
Constit. of *Nassauvia magellanica*. Oil.

Bittner, M. *et al*, *Phytochemistry*, 1988, **27**, 3845.

Isovolubilin I-80098

6-(6-Deoxy-α-L-mannopyranosyl)-5-hydroxy-7-methoxy-3-(4-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI. 7-O-Methylbiochanin A 6-C-rhamnoside. 5-Hydroxy-4',7-dihydroxy-6-rhamnosylisoflavone

[56317-19-2]



$C_{23}H_{24}O_9$ M 444.437

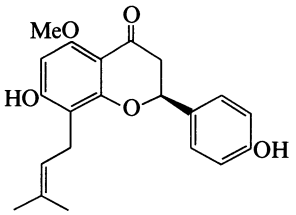
Isol. from flowers of *Dalbergia volubilis*. Hemihydrate. Mp 298-301°. $[\alpha]_D^{30}$ +17° (c, 1.15 in MeOH).

Chawla, H.M. *et al*, *Indian J. Chem.*, 1975, **13**, 444.

Isoxanthohumol† I-80099

Updated Entry replacing I-01631

4′,7-Dihydroxy-5-methoxy-8-C-prenylflavanone. Humulol[+]



$C_{21}H_{22}O_5$ M 354.402

The name Humulol has historical precedence but Isoxanthohumol has been preferred to avoid confusion with I-01631. However another nat. prod. has since been named Isoxanthohumol; not i see I-80100.

(S)-form [70872-29-6]

Isol. from hop (*Humulus lupulus*). Light yellow needles (AcOH). Mp 198°.

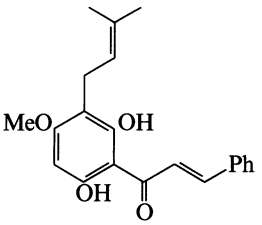
Di-Me ether: Mp 174-175°.

Power, F.B. *et al*, *J. Chem. Soc.*, 1913, **103**, 1267 (*isol*)
Verzele, M. *et al*, *Bull. Soc. Chim. Belg.*, 1957, **66**, 452 (*isol*)
Jain, A.C. *et al*, *Tetrahedron*, 1978, **34**, 3563 (*synth*)

Isoxanthohumol† I-80100

1-[2,6-Dihydroxy-4-methoxy-3-(3-methyl-2-butenyl)phenyl]-3-phenyl-2-propen-1-one. 2′,6′-Dihydroxy-4′-methoxy-3′-prenylchalcone

[72247-79-1]



$C_{21}H_{22}O_4$ M 338.402

Not the same as Isoxanthohumol†, I-80099. The name Isoxanthohumol is misleading; not isomeric with X-00027 which has an addnl. OH group. Isol. from *Helichrysum cymosum*. Yellowish oil.

O-*De-Me:* [72247-78-0]. ***Desmethylxanthohumol***

$C_{20}H_{20}O_4$ M 324.376

Isol. from roots of *Helichrysum tenuiculum*. Yellow cryst. (Et_2O). Mp 168-169°. Incorrectly named. See above.

Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 1033.

4-Isoxazolecarboxylic acid I-80101

Updated Entry replacing I-01635

$C_4H_3NO_3$ M 113.073

Plates (toluene), cryst. ($CHCl_3$ or by subl.). Mp 123-124° (121-123°). Dec. at 140° or on keeping.

Et ester:

$C_6H_7NO_3$ M 141.126

Liq. Bp_{13-14} 93°.

Nitrile: [68776-58-9]. *4-Cyanoisoxazole*

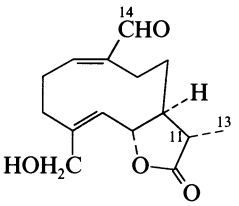
$C_4H_2N_2O$ M 94.073

Sticky pale yellow solid.

Panizzi, L., *Gazz. Chim. Ital.*, 1947, **77**, 206 (*synth, ester*)
Maggioni, P. *et al*, *Gazz. Chim. Ital.*, 1966, **96**, 443 (*synth, ir*)
Angus, R.O. *et al*, *Synthesis*, 1988, 746 (*nitrile*)

Ixerin A I-80102

[91486-96-3]



$C_{15}H_{20}O_4$ M 264.321

Isol. from *Ixera tamagawensis*. Prisms (MeOH). Mp 134-138°. $[\alpha]_D^{23}$ −54.6° (c, 0.18 in $CHCl_3$).

O-*β-D-Glucopyranoside:* [94356-09-9]. ***Ixerin J***

$C_{21}H_{30}O_9$ M 426.463

Constit. of *I. tamagawensis*. Prisms. Mp 113.5-115.5°. $[\alpha]_D^{25}$ −54.0° (c, 0.68 in MeOH).

14-Alcohol: [91486-99-6]. ***Ixerin K***

$C_{15}H_{22}O_4$ M 266.336

Constit. of *I. tamagawensis*. Amorph. powder. $[\alpha]_D^{25}$ −40.6° (c, 0.62 in MeOH).

14-Alcohol, 11-epimer: [94356-08-8]. ***Ixerin L***

$C_{15}H_{22}O_4$ M 266.336

Constit. of *I. tamagawensis*. Amorph. powder. $[\alpha]_D^{25}$ +23.5° (c, 0.37 in MeOH).

11,13-Didehydro: ***8-Desoxyurospermal A***

$C_{15}H_{18}O_4$ M 262.305

Isol. from *I. tamagawensis*. Amorph. powder. $[\alpha]_D^{23}$ −40.6° (c, 0.32 in $CHCl_3$).

11,13-Didehydro, 15-O-β-D-glucopyranoside: [91486-97-4]. ***Ixerin B***

$C_{21}H_{28}O_9$ M 424.447

Constit. of *I. tamagawensis*. Amorph. $[\alpha]_D^{23}$ −11.9° (c, 2.0 in MeOH).

11,13-Didehydro, 15-O-β-D-(6-O-p-hydroxyphenylacetyl)glucopyranoside: [91486-98-5]. ***Ixerin C***

$C_{29}H_{34}O_{11}$ M 558.581

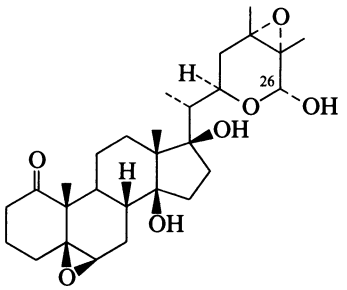
Constit. of *I. tamagawensis*. Amorph. $[\alpha]_D^{23}$ +3.8° (c, 0.40 in MeOH).

Asada, H. *et al*, *Chem. Pharm. Bull.*, 1984, **32**, 3403.

J

Jaborosalactol *M* — J-80001

[120160-86-3]



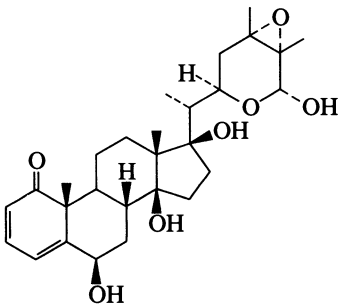
$C_{28}H_{42}O_7$ M 490.636
Constit. of *Jaborosa bergii*. Cryst. (EtOAc). Mp 234-236°.

26-Ketone: [120160-85-2]. ***Jaborosalactone* M**
$C_{28}H_{40}O_7$ M 488.620
Constit. of *J. bergii*.

Monteagudo, E.S. *et al*, *Phytochemistry*, 1988, **27**, 3925.

Jaborosalactol N — J-80002

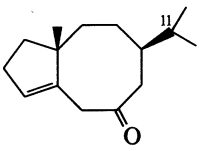
[120160-87-4]



$C_{28}H_{40}O_7$ M 488.620
Constit. of *Jaborosa bergii*. Cryst. (EtOAc). Mp 183-185° dec.

Monteagudo, E.S. *et al*, *Phytochemistry*, 1988, **27**, 3925.

Jasionone — J-80003



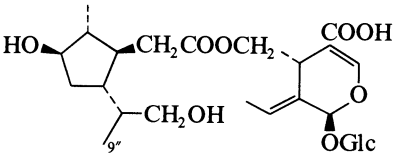
$C_{15}H_{24}O$ M 220.354
Parent compd. apparently unknown.

11-Hydroxy: [119765-85-4]. *11-Hydroxyjasionone*
$C_{15}H_{24}O_2$ M 236.353
Constit. of *Jasonia montana*. Oil.

Ahmed, A.A. *et al*, *Phytochemistry*, 1988, **27**, 3875.

Jasmesosidic acid — J-80004

Updated Entry replacing J-50009



$C_{26}H_{40}O_{13}$ M 560.594

Me ester: [97777-70-3]. ***Jasmesoside***
$C_{27}H_{42}O_{13}$ M 574.621
Constit. of *Jasminum mesnyi*. Powder. $[\alpha]_D^{24}$ −156° (c, 0.73 in MeOH).

9″-Hydroxy: ***9″-Hydroxyjasmesosidic acid***
$C_{26}H_{40}O_{14}$ M 576.594
Constit. of *J. mesnyi*. Powder. $[\alpha]_D$ −161° (c, 0.65 in MeOH).

9″-Hydroxy, Me ester: ***9″-Hydroxyjasmesoside***
$C_{27}H_{42}O_{14}$ M 590.620
Constit. of *J. mesnyi*. Powder. $[\alpha]_D$ −164.9° (c, 0.49 in MeOH).

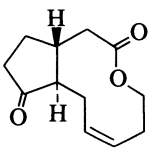
Inoue, K. *et al*, *Phytochemistry*, 1985, **24**, 1299 (*isol*, *struct*)
Tanahashi, T. *et al*, *Phytochemistry*, 1989, **28**, 1413 (*isol*, *struct*)

Jasmine ketolactone — J-80005

Updated Entry replacing J-40003

*1,4,5,8,8*a*,10,11,11*a*-Octahydrocyclopent*[d]*oxecin-2,9-dione, 9CI. Jasmine oil ketolactone*

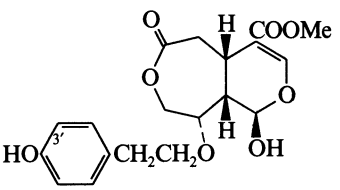
[70981-24-7]



$C_{12}H_{16}O_3$ M 208.257
Constit. of Italian jasmine oil (*Jasminium grandiflorum*). Small needles (pet. ether). Mp 104°. $[\alpha]_D^{20}$ −260° (c, 3.05 in MeOH).

Demole, E. *et al*, *Helv. Chim. Acta*, 1964, **47**, 1152 (*isol*, *ir*, *pmr*, *ms*, *struct*)
Kitahara, T. *et al*, *Agric. Biol. Chem.*, 1984, **48**, 1731 (*synth*)

Jasmolactone A — J-80006



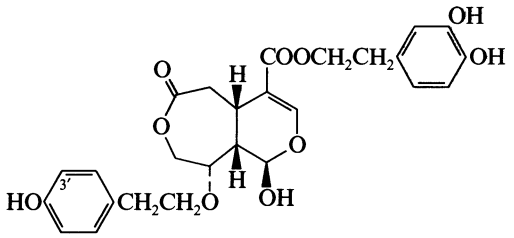
$C_{19}H_{22}O_8$ M 378.378
Constit. of *Jasminum multiflorum*. Pale yellow solid. $[\alpha]_D^{28}$ +122.4° (c, 1 in $CHCl_3$).

3′-Hydroxy: ***Jasmolactone B***
$C_{19}H_{22}O_9$ M 394.377

Constit. of *J. multiflorum*. Pale yellow gum. $[\alpha]_D^{28}$ +100.1° (c, 0.1 in MeOH).

Shen, Y.-C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1060 (*isol, pmr, cmr*)

Jasmolactone C J-80007



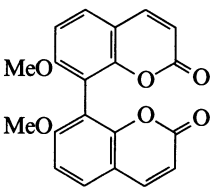
$C_{26}H_{28}O_{10}$ M 500.501
Constit. of *Jasmium multiflorum*. Gum. $[\alpha]_D^{28}$ +48.6° (c, 1 in MeOH).

3'-Hydroxy: ***Jasmolactone D***
Constit. of *J. multiflorum*. Gum. $[\alpha]_D^{28}$ +28.5° (c, 1 in MeOH).

Shen, Y.-C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1060 (*isol, pmr, cmr*)

Jayantinin J-80008

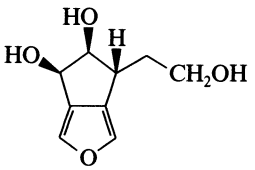
7,7'-Dimethoxy-8,8'-bi[2H-1-benzopyran-2-one]. 7,7'-Dimethoxy-8,8'-bicoumarin



$C_{20}H_{14}O_6$ M 350.327
Constit. of *Boenninghausenia albiflora*. Green powder. Mp 255-256°.

Joshi, P.C. *et al*, *Phytochemistry*, 1989, **28**, 1281.

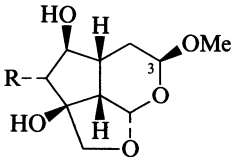
Jiofuran J-80009



$C_9H_{12}O_4$ M 184.191
Constit. of *Rehmannia glutinosa*. Amorph. powder. $[\alpha]_D^{24}$ −30.4° (c, 0.19 in MeOH).

Morota, T. *et al*, *Phytochemistry*, 1989, **28**, 2385 (*isol, pmr, cmr*)

Jioglutin A J-80010



R = Cl

$C_{10}H_{15}ClO_5$ M 250.678
Constit. of *Rehmannia glutinosa*. Amorph. powder. $[\alpha]_D$ +63.3° (c, 1 in MeOH).

3-Epimer: ***Jioglutin B***
$C_{10}H_{15}ClO_5$ M 250.678
Constit. of *Rehmannia glutinosa*. Amorph. powder. $[\alpha]_D$ −63.2° (c, 0.94 in MeOH).

Morota, T. *et al*, *Phytochemistry*, 1989, **28**, 2385 (*isol, pmr, cmr*)

Jioglutin C J-80011

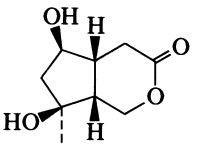
As Jioglutin A, J-80010 with

R = OH

$C_{10}H_{16}O_6$ M 232.233
Constit. of *Rehmannia glutinosa*. Amorph. powder. $[\alpha]_D$ +58.1° (c, 0.89 in MeOH).

Morota, T. *et al*, *Phytochemistry*, 1989, **28**, 2385 (*isol, pmr, cmr*)

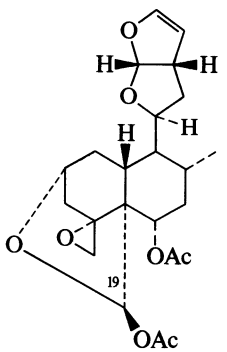
Jioglutolide J-80012



$C_9H_{14}O_4$ M 186.207
Constit. of *Rehmannia glutinosa*. Needles (Me_2CO). Mp 141-142°. $[\alpha]_D$ −8.4° (c, 1.19 in MeOH).

Morota, T. *et al*, *Phytochemistry*, 1989, **28**, 2385 (*isol, pmr, cmr, cryst struct*)

Jodrellin A J-80013



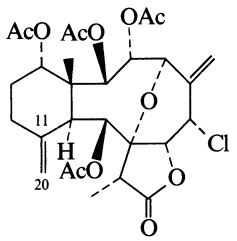
$C_{24}H_{32}O_8$ M 448.512
Constit. of *Scutellaria woronowii*. Insect antifeedant. Oil.

19-De-Ac, 19-O-(2-methylpropanoyl): ***Jodrellin B***
$C_{26}H_{36}O_8$ M 476.566
Constit. of *S. woronowii*. Insect antifeedant. Oil. $[\alpha]_D^{20}$ −11.4° (c, 0.07 in $CHCl_3$).

Anderson, J.C. *et al*, *Tetrahedron Lett.*, 1989, **30**, 4737.

Junceellin J-80014

[92508-09-3]



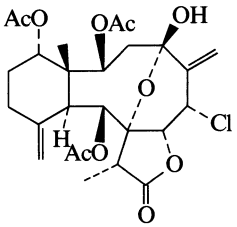
$C_{28}H_{35}ClO_{11}$ M 583.031
Constit. of gorgonians *Junceella squamata* and *J. fragilis*.

11α,20-Epoxide: [86425-67-4]. ***Praelolide***
$C_{28}H_{35}ClO_{12}$ M 599.030
Constit. of *Plexaureides praelonga* and *J. fragilis*.

Dai, J. *et al*, *Sci. Sin.* (*Engl. Ed.*), 1985, **28**, 1131.
Shin, J. *et al*, *Tetrahedron*, 1989, **45**, 1633.

Junceellolide A J-80015

[121769-81-1]

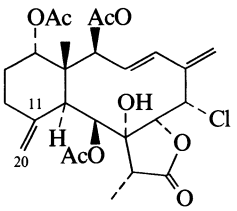


$C_{26}H_{33}ClO_{10}$ M 540.993
Constit. of gorgonian *Junceella fragilis*. Cryst. Mp 115-116°. $[\alpha]_D$ −7.9° (c, 0.6 in $CHCl_3$).

Shin, J. *et al*, *Tetrahedron*, 1989, **45**, 1633.

Junceellolide B J-80016

[121798-80-9]



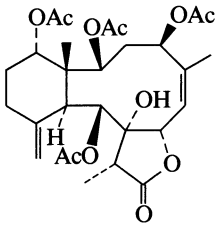
$C_{26}H_{33}ClO_9$ M 524.994
Constit. of *Junceella fragilis*. Cryst. Mp 95-96°. $[\alpha]_D$ +9.4° (c, 1.3 in $CHCl_3$).

11α,20-Epoxide: [121769-82-2]. ***Junceellolide C***
$C_{26}H_{33}ClO_{10}$ M 540.993
Constit. of *J. fragilis*. Cryst. Mp 120-125°. $[\alpha]_D$ +36.1° (c, 1.2 in $CHCl_3$).

Shin, J. *et al*, *Tetrahedron*, 1989, **45**, 1633.

Junceellolide D J-80017

[121798-81-0]



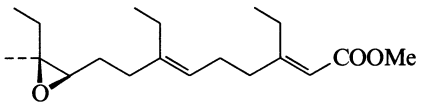
$C_{28}H_{38}O_{11}$ M 550.602
Constit. of *Junceella fragilis*. Cryst. Mp 208-209°. $[\alpha]_D$ −7.7° (c, 2.5 in $CHCl_3$).

Shin, J. *et al*, *Tetrahedron*, 1989, **45**, 1633.

Juvenile hormone O J-80018

Methyl 10,11-epoxy-3,7-diethyl-11-methyl-2,6-tridecadienoate

[117019-48-4]



$C_{19}H_{32}O_3$ M 308.460
Isol. from developing embryos of the tobacco hornworm moth *Manduca sexta*. Part of the juvenile hormone complex essential to the devolopment of insects. Oil. $[\alpha]_D^{18}$ +13.8° (c, 0.92 in MeOH). n_D^{18} 1.4752. The nat. hormone is known to be (*E*,*E*) but the abs. config. of the epoxide function is currently unknown. The synthetic prod. was (10*R*, 11*S*) as shown.

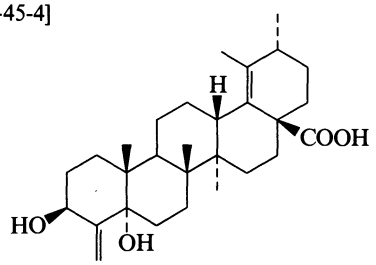
Mori, K. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 41.

K

Kanerin **K-80001**

3β,5α-Dihydroxy-24-nor-4(23),18-ursadien-28-oic acid, 9CI

[120396-45-4]



$C_{29}H_{44}O_4$ M 456.664

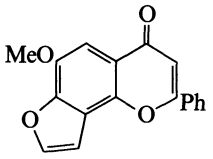
Constit. of leaves of *Nerium oleander*. Cryst. (MeOH). Mp 280-281°. $[\alpha]_D$ +14.28° (c, 0.14 in $CHCl_3$).

Siddiqui, S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 57 (*isol, pmr, cmr*)

Kanjone **K-80002**

*6-Methoxy-2-phenyl-4*H*-furo[2,3-*h*]-1-benzopyran-4-one, 9CI. 6-Methoxyfuro[2,3-*h*]flavone*

[1094-12-8]



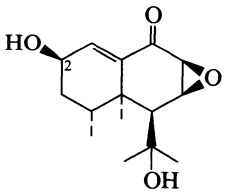
$C_{18}H_{12}O_4$ M 292.290

Isol. from seeds of *Pongamia glabra*. Cryst. (MeOH). Mp 190-191°.

Aneja, R. *et al*, *J. Chem. Soc.*, 1963, 163 (*isol, uv, ir, synth*)
Talapatra, K.S. *et al*, *J. Indian Chem. Soc.*, 1982, **59**, 534 (*cmr*)

Kanshone D **K-80003**

[119403-26-8]



$C_{15}H_{22}O_4$ M 266.336

Constit. of *Nardostachys chinensis*. Needles. Mp 152-153°. $[\alpha]_D$ +57.9° (c, 0.52 in $CHCl_3$).

2-Ketone: [119403-27-9]. ***Kanshone E***

$C_{15}H_{20}O_4$ M 264.321

Constit. of *N. chinensis*. Gum. $[\alpha]_D$ −42.2° (c, 1.29 in $CHCl_3$).

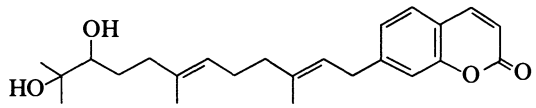
Bagchi, A. *et al*, *Phytochemistry*, 1988, **27**, 3667.

Karatavicinol **K-80004**

Updated Entry replacing K-00021

*7-[(10,11-Dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl)oxy]-2*H*-1-benzopyran-2-one, 9CI. 7-(10,11-Dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl)coumarin. Karatavikinol*

[25374-66-7]



$C_{24}H_{32}O_4$ M 384.514

Constit. of the root of *Ferula karatavica*. Mp 52-53°. $[\alpha]_D^{20}$ −12° (c, 7.5 in EtOH).

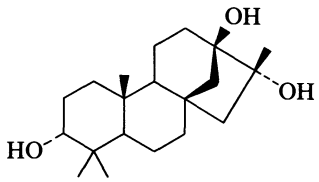
10-O-β-Sophoroside: [53011-70-4]. ***Reoselin A.*** *Reoselin*

$C_{36}H_{52}O_{15}$ M 724.798

Isol. from *F. pseudooreoselinum* and *F. korshinskyi*. Mp 160-161° (155-156°). $[\alpha]_D$ −73.5° (MeOH), $[\alpha]_D$ −24.4° (EtOH).

Kir'yalov, N.P. *et al*, *Khim. Prir. Soedin.*, 1969, **5**, 225; 1974, **10**, 84; 1975, **11**, 87; *Chem. Nat. Compd.*, pp. 191, 82, 88.

3,13,16-Kauranetriol **K-80005**



$C_{20}H_{34}O_3$ M 322.487

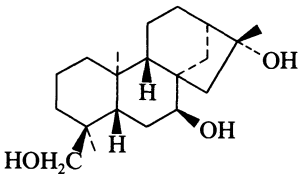
(3α,16α)-form

Constit. of *Agathis vitiensis*. Needles (EtOAc). Mp 124-126°.

Cambie, R.C. *et al*, *Phytochemistry*, 1989, **28**, 1675.

***ent*-7α,16β,18-Kauranetriol** **K-80006**

Distanol

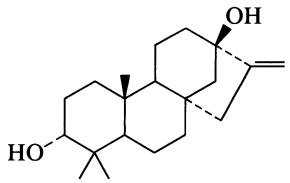


$C_{20}H_{34}O_3$ M 322.487

Constit. of *Sideritis distans*. Cryst. (EtOAc). Mp 260-265°.

Venturella, P. *et al*, *Phytochemistry*, 1989, **28**, 1976.

16-Kaurene-3,13-diol K-80007



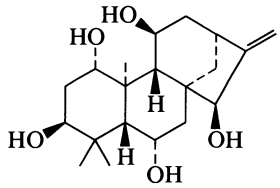
$C_{20}H_{32}O_2$ M 304.472

3α-form

Constit. of *Agathis vitiensis*. Needles (EtOAc). Mp 205-208°. $[\alpha]_D^{17}$ +28° (c, 1 in MeOH).

Cambie, R.C. *et al*, *Phytochemistry*, 1989, **28**, 1675.

ent-16-Kaurene-1β,3α,6β,11α,15α-pentol K-80008



$C_{20}H_{32}O_5$ M 352.470

1,3-Di-Ac: ent-1β,3α-*Diacetoxy*-16-*kaurene*-6β,11α,15α-*triol*. ***Inflexarabdonin A***

$C_{24}H_{36}O_7$ M 436.544

Constit. of *Rabdosia inflexa*. Cryst. ($CHCl_3$/hexane). Mp 118-120°. $[\alpha]_D^{27.5}$ −5.5° (c, 1.95 in MeOH).

6-Ketone, 1,3-Di-Ac: ent-1β,3α-*Diacetoxy*-11α,15α-*dihydroxy*-16-*kauren*-6-*one*. ***Inflexarabdonin B***

$C_{24}H_{34}O_7$ M 434.528

Constit. of *R. inflexa*. Amorph. powder. $[\alpha]_D^{24}$ −16.9° (c, 0.83 in MeOH).

Takeda, Y. *et al*, *Phytochemistry*, 1989, **28**, 851.

ent-15-Kauren-18-oic acid K-80009

Isokaurenic acid

$C_{20}H_{30}O_2$ M 302.456

Isol. from resin of *Trachylobium verrucosum*.

Me ester: Cryst. (Et_2O/MeOH). Mp 123°. $[\alpha]_D$ ±0° (c, 1.2 in $CHCl_3$).

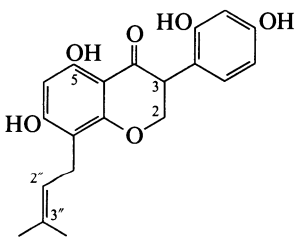
Hugel, G. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1974; 1965, 2882, 2888 (*isol*, *ir*, *pmr*, *ms*, *struct*)

Kievitone K-80010

Updated Entry replacing K-00113

*3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI. 8-(3,3-Dimethylallyl)-2′,4′,5,7-tetrahydroxyisoflavanone. 2′,4′,5,7-Tetrahydroxy-8-*C*-prenylisoflavone. Vignatin. Phaseolus substance II*

[40105-60-0]



$C_{20}H_{20}O_6$ M 356.374

Isol. from *Dolichos biflorus*, *Lablab niger*, *Macroptilium atropurpureum*, *Macrotyloma axillare*, *Mucuna utilis*, *Phaseolus aureus*, *P. calcaratus*, *P. lunatus*, *P. vulgaris*, *Stizolobium deeringianum* and *Vigna unguiculata* (all Leguminosae, Papilionoideae).

2,3-Didehydro: [74161-25-4]. ***2,3-Dehydrokievitone***

$C_{20}H_{18}O_6$ M 354.359

Isol. from pods of *P. vulgaris*.

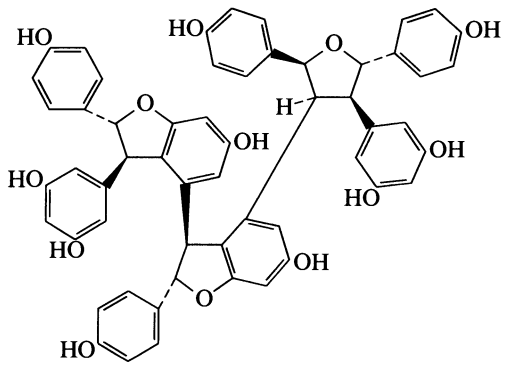
5-Deoxy: [74161-24-3]. ***5-Deoxykievitone***

$C_{20}H_{20}O_5$ M 340.375

Isol. from pods of *P. vulgaris*.

Burden, R.S. *et al*, *Tetrahedron Lett.*, 1972, 4175 (*isol*)
Smith, D.A. *et al*, *Physiol. Plant Pathol.*, 1973, **3**, 293 (*ms*, *ir*, *uv*)
Granamanickam, S.S., *Experientia*, 1979, **35**, 323 (*isol*)
Woodward, M.D., *Phytochemistry*, 1979, **18**, 2007 (2,3-*Dehydrokievitone*, 5-*Deoxykievetone*)
Woodward, M.D., *Phytochemistry*, 1979, **18**, 363 (*occur*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev*, *occur*)

Kobophenol A K-80011



$C_{56}H_{44}O_{13}$ M 924.956

Constit. of *Carex kobomugi*. Pale yellow oil. $[\alpha]_D^{20}$ +227° (c, 0.17 in MeOH).

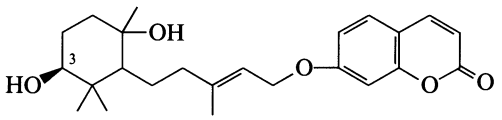
Kawabata, J. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3785.

Kopeolin K-80012

Updated Entry replacing K-00148

*7-[[5-(3,6-Dihydroxy-2,2,6-trimethylcyclohexyl)-3-methyl-2-pentyl]oxy]-2*H*-1-benzopyran-2-one, 9CI*

[51005-86-8]



$C_{24}H_{32}O_5$ M 400.514

Constit. of the roots of *Ferula kopetdaghensis*. Cryst. (C_6H_6). Mp 146-147°. $[\alpha]_D^{25}$ −15.9° (c, 0.98 in EtOH).

3-O-β-D-Glucopyranoside: [50982-41-7]. ***Kopeoside***

$C_{30}H_{42}O_{10}$ M 562.656

Constit. of *F. kopetdaghensis*. Cryst. (MeOH aq.). Mp 177-178°. $[\alpha]_D^{25}$ −22.1° (c, 1.47 in EtOH).

3-Ketone: [81758-04-5]. ***Kopeolone***

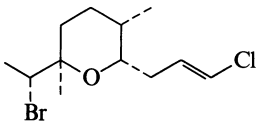
$C_{24}H_{30}O_5$ M 398.498

Constit. of *F. kopetdaghensis*. Cryst. Mp 125-126°. $[\alpha]_D$ +170° (c, 1 in EtOH).

Kamilov, Kh.M. *et al*, *Khim. Prir. Soedin.*, 1973, 308; *CA*, **79**, 134321 (*isol*)
Nabiev, A.A. *et al*, *Khim. Prir. Soedin.*, 1982, **18**, 48 (*Kopeolone*)

Kumepaloxane K-80013

[122666-10-8]

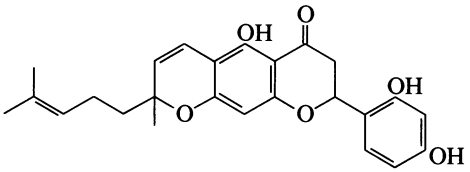


$C_{12}H_{20}BrClO$ M 295.646

Constit. of bubble shell *Haminoea cymbalum*. Fish antifeedant. Oil. $[\alpha]_D$ +22.6° (c, 0.32 in $CHCl_3$).

Poiner, A. *et al*, *Tetrahedron*, 1989, **45**, 617.

Kuwanol C K-80014

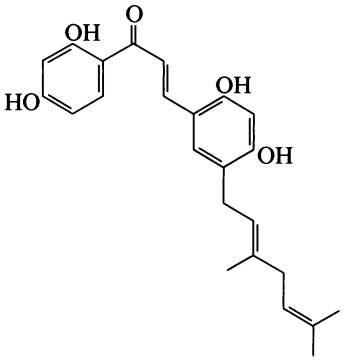


$C_{25}H_{26}O_6$ M 422.477

Constit. of *Morus alba*. Amorph. powder. $[\alpha]_D^{22}$ −10° (c, 0.31 in EtOH).

Hano, Y. *et al*, *Heterocycles*, 1989, **29**, 807.

Kuwanol D K-80015



$C_{25}H_{28}O_5$ M 408.493

Constit. of *Morus alba*. Yellow amorph. powder.

Hano, Y. *et al*, *Heterocycles*, 1989, **29**, 807.

L

7,14-Labdadiene-3,13-diol — L-80001

$C_{20}H_{34}O_2$ M 306.487

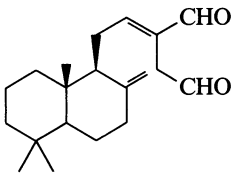
(3α,13R)-form

Constit. of *Waitzia acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

8(17),12-Labdadiene-15,16-dial — L-80002

[104263-88-7]



$C_{20}H_{30}O_2$ M 302.456

Constit. of *Curcuma heyneana*. Oil. $[\alpha]_D^{20}$ +16° (c, 0.23 in MeOH).

Firman, K. *et al*, *Phytochemistry*, 1988, **27**, 3887.

ent-7,13-Labdadiene-2α,15-diol — L-80003

$C_{20}H_{34}O_2$ M 306.487

Constit. of *Ophryosporus heptanthus*. Gum.

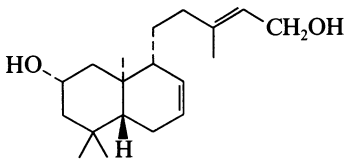
15-Ac: ent-15-*Acetoxy*-7,13-*labdadien*-2α-*ol*

$C_{22}H_{36}O_3$ M 348.525

Constit. of *O. heptanthus*. Gum.

Ferracini, V.L. *et al*, *Phytochemistry*, 1989, **28**, 1463.

ent-7,13-Labdadiene-2β,15-diol — L-80004



$C_{20}H_{34}O_2$ M 306.487

Constit. of *Baccharis sternbergiana*. Oil. $[\alpha]_D^{24}$ −5° (c, 0.8 in $CHCl_3$).

15-Ac: ent-15-*Acetoxy*-7,13-*labdadien*-2β-*ol*

$C_{22}H_{36}O_3$ M 348.525

Constit. of *B. sternbergiana*. Oil. $[\alpha]_D^{24}$ −9.5° (c, 2.13 in $CHCl_3$).

2-Ketone: ent-15-*Hydroxy*-7,13-*labdadien*-2-*one*

$C_{20}H_{32}O_2$ M 304.472

Constit. of *B. sternbergiana*.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

8,14-Labdadiene-2,3,7,13,20-pentol — L-80005

$C_{20}H_{34}O_5$ M 354.486

(2α,3α,7α,13R)-form

*2-Angeloyl, 3,20-di-Ac: 3α,20-Diacetoxy-2α-angeloyloxy-*8,14-*labdadiene*-7α,13R-*diol*

$C_{29}H_{44}O_8$ M 520.662

Constit. of *Waitzia acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

8(17),14-Labdadiene-2,3,7,13,20-pentol — L-80006

$C_{20}H_{34}O_5$ M 354.486

(2α,3α,7α,13R)-form

2-Angeloyl, 20-Ac: 20-Acetoxy-2α-angeloyloxy-8(17),14-*labdadiene*-3α,7α,13R-*triol*

$C_{27}H_{42}O_7$ M 478.625

Constit. of *Waitzia acuminata*.

2-Angeloyl, 20-(2-methylbutanoyl): 2α-Angeloyloxy-20-(2-*methylbutanoyloxy*)-8(17),14-*labdadiene*-3α,7α,13R-*triol*

$C_{30}H_{48}O_7$ M 520.705

Constit. of *W. acuminata*.

*2-Angeloyl, 3,20-di-Ac: 3α,20-Diacetoxy-2α-angeloyloxy-*8(17),14-*labdadiene*-7α,13R-*diol*

$C_{29}H_{44}O_8$ M 520.662

Constit. of *W. acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

7,14-Labdadiene-2,3,13,20-tetrol — L-80007

$C_{20}H_{34}O_4$ M 338.486

(2α,3α,13R)-form

2-Angeloyl, 20-Ac: 20-Acetoxy-2α-angeloyloxy-7,14-*labdadiene*-3α,13R-*diol*

$C_{27}H_{42}O_6$ M 462.625

Constit. of *Waitzia acuminata*.

2-Angeloyl, 20-(2-methylbutanoyl): 2α-Angeloyloxy-20-(2-*methylbutanoyloxy*)-7,14-*labdadiene*-3α,13S-*diol*

$C_{30}H_{48}O_6$ M 504.706

Constit. of *W. acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

8(17),14-Labdadiene-2,7,13,20-tetrol — L-80008

$C_{20}H_{34}O_4$ M 338.486

(2α,7α,13R)-form

2-Angeloyl, 20-Ac: 20-Acetoxy-2α-angeloyloxy-8(17),14-*labdadiene*-7α,13R-*diol*

$C_{27}H_{42}O_6$ M 462.625

Constit. of *Waitzia acuminata*.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

ent-7,13-Labdadiene-2β,3β,15-triol — L-80009

$C_{20}H_{34}O_3$ M 322.487

Constit. of *Baccharis sternbergiana*.

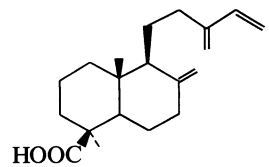
Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

8(17),13(16),14-Labdatrien-19-oic acid — L-80010

Updated Entry replacing L-00040

Myrceocommunic acid. $\Delta^{13(16)}$-*Communic acid*

[31323-66-7]



$C_{20}H_{30}O_2$ M 302.456

Constit. of *Callitris columellaris* and *Juniperus oxycedrus*. Cryst. (MeOH). Mp 129-130° (115-117°). $[\alpha]_D$ +53.6° ($CHCl_3$).

19-Aldehyde: [56709-03-6]. *8(17),13(16),14-Labdatrien-19-al.* ***Myrceocommunal***
$C_{20}H_{30}O$ M 286.456
Isol. from *J. oxycedrus*.

Atkinson, P.W. *et al*, *Tetrahedron*, 1970, **26**, 1935 (*isol, ms*)
Carman, R.M. *et al*, *Aust. J. Chem.*, 1971, **24**, 353 (*isol, pmr*)
Teresa, J.P. *et al*, *An. Quim.*, 1972, **68**, 1061; 1978, **74**, 966 (*isol*)

7-Labdene-15,17-dioic acid L-80011

$C_{20}H_{32}O_4$ M 336.470
Constit. of *Halimium verticillatum*.

Di-Me ester: Oil. $[\alpha]_D^{22}$ −21.8° (c, 0.77 in $CHCl_3$).

Urones, J.G. *et al*, *Phytochemistry*, 1989, **28**, 557.

7-Labdene-15,17-diol L-80012

$C_{20}H_{36}O_2$ M 308.503

Di-Ac: 15,17-Diacetoxy-7-labdene
$C_{24}H_{40}O_4$ M 392.578
Constit. of *Halimium verticillatum*. Oil. $[\alpha]_D^{22}$ −9.7° (c, 0.83 in $CHCl_3$).

Urones, J.G. *et al*, *Phytochemistry*, 1989, **28**, 557.

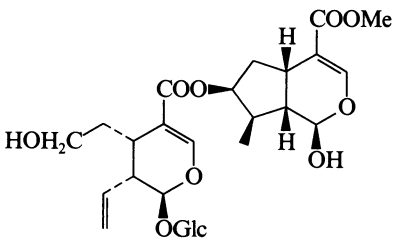
8(20)-Labdene-3,15-diol L-80013

$C_{20}H_{36}O_2$ M 308.503

3β-form
Isol. from *Araucaria imbricata*. Platelets (pet. ether). Mp 114°. $[\alpha]_D$ +29° (c, 0.6 in $CHCl_3$).

Chandra, G. *et al*, *J. Chem. Soc.*, 1964, 3648 (*isol, uv, ir, ms*)

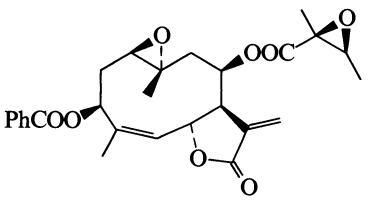
Laciniatoside V L-80014



$C_{27}H_{38}O_{14}$ M 586.589
Constit. of *Dipsacus laciniatus*. Amorph. $[\alpha]_D^{27}$ −98° (c, 0.67 in MeOH).

Podányi, B. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 135 (*isol, pmr, cmr*)

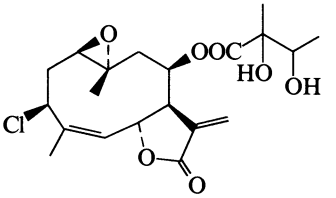
Lacinolide A L-80015



$C_{27}H_{30}O_8$ M 482.529
Constit. of *Viguiera laciniata*. Cryst.

Gao, F. *et al*, *Phytochemistry*, 1989, **28**, 2409 (*isol, pmr, cmr, cryst struct*)

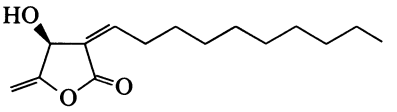
Lacinolide B L-80016



$C_{20}H_{27}ClO_7$ M 414.882
Constit. of *Viguiera laciniata*.

Gao, F. *et al*, *Phytochemistry*, 1989, **28**, 2409 (*isol, pmr, cmr*)

Lancifolide L-80017



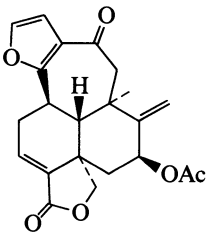
$C_{15}H_{24}O_3$ M 252.353
Constit. of *Actinodaphne lancifolia*. Oil. $[\alpha]_D$ −49.0° (c, 0.58 in $CHCl_3$).

E-*Isomer:* ***Isolancifolide***
$C_{15}H_{24}O_3$ M 252.353
Constit. of *A. lancifolia*. Oil. $[\alpha]_D$ −59.0° (c, 0.5 in $CHCl_3$).

Tanaka, H. *et al*, *Phytochemistry*, 1989, **28**, 626.

Languiduline L-80018

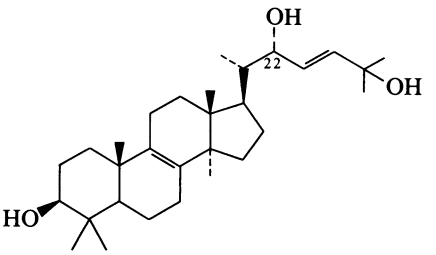
[114391-81-0]



$C_{22}H_{22}O_6$ M 382.412
Constit. of *Salvia languidula*. Cryst. Mp 243-245°. $[\alpha]_D^{20}$ −193.4° (c, 0.2 in $CHCl_3$).

Córdenas, J. *et al*, *Heterocycles*, 1988, **27**, 1809 (*isol, cryst struct, cmr*)

8,23-Lanostadiene-3,22,25-triol L-80019



$C_{30}H_{50}O_3$ M 458.723

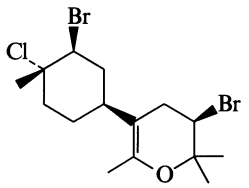
(3α,22S,23E)-form

22-Ac: [119513-66-5]. *22-Acetoxy-8,23-lanostadiene-3α,25-diol*
$C_{32}H_{52}O_4$ M 500.760
Metab. of *Pisolithus tinctorius*. Cryst. (MeOH). Mp 187-190°.

3,22-Di-Ac: Cryst. (MeOH). Mp 190-192°. $[\alpha]_D$ +6° (c, 1.5 in $CHCl_3$).

Lobo, A.M. *et al*, *Phytochemistry*, 1988, **27**, 3569 (*isol, cryst struct*)

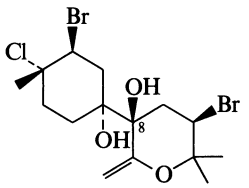
Laucopyranoid A L-80020



$C_{15}H_{23}Br_2ClO$ M 414.607
Constit. of *Laurencia caespitosa*. Cryst. Mp 118-120°. $[\alpha]_D$ +0.5° (c, 0.87 in $CHCl_3$).

Chang, M. *et al*, *Phytochemistry*, 1989, **28**, 1417.

Laucopyranoid B L-80021

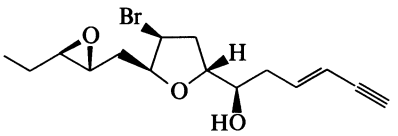


$C_{15}H_{23}Br_2ClO_2$ M 430.606
Constit. of *Laurencia caespitosa*. Cryst. Mp 97-98°. $[\alpha]_D$ +11.0° (c, 1.12 in $CHCl_3$).

8-Epimer: ***Laucopyranoid C***
$C_{15}H_{23}Br_2ClO_2$ M 430.606
Constit. of *L. caespitosa*. Unstable.

Chang, M. *et al*, *Phytochemistry*, 1989, **28**, 1417.

Laureoxolane L-80022

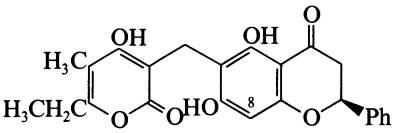


$C_{15}H_{21}BrO_3$ M 329.233
Metab. of *Laurencia nipponica*. Unstable oil. $[\alpha]_D^{24}$ +21.9° (c, 0.32 in $CHCl_3$).

Fukuzawa, A. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3665.

Lepidissipyrone L-80023

[122585-68-6]



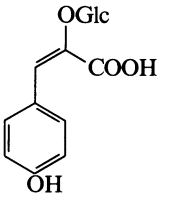
$C_{24}H_{22}O_7$ M 422.434
Constit. of *Helichrysum lepidissimum*. Gum.

8-(3-Methyl-2-butenyl): [122616-68-6]. ***8-Prenyllepidissipyrone***
$C_{29}H_{30}O_7$ M 490.552
Constit. of *H. lepidissimum*. Gum.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

Lespedezic acid L-80024

[123955-02-2]



$C_{15}H_{18}O_9$ M 342.302
Constit. of *Lesperzeza cuneata*. Leaf-opening factor. Powder (as K salt). $[\alpha]_D^{25}$ −57.4° (c, 0.65 in H_2O).

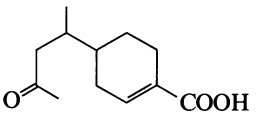
Z-Isomer: [123955-03-3]. ***Isolespedezic acid***
$C_{15}H_{18}O_9$ M 342.302
Constit. of *L. cuneata*. Powder (as K salt). $[\alpha]_D^{25}$ +53.1° (c, 1.0 in H_2O).

Shigemori, H. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3991.

Libanotic acid L-80025

4-(1-Methyl-3-oxobutyl)-1-cyclohexene-1-carboxylic acid, 9CI. 11,12,13-Trinor-9-oxo-2-bisabolen-15-oic acid

[119765-97-8]

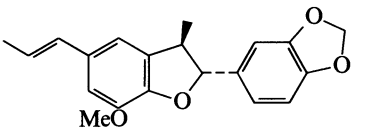


$C_{12}H_{18}O_3$ M 210.272
Constit. of *Cedrus libani*. Oil.

Avcibasi, H. *et al*, *Phytochemistry*, 1988, **27**, 3967.

Licarin E L-80026

[51020-87-2]



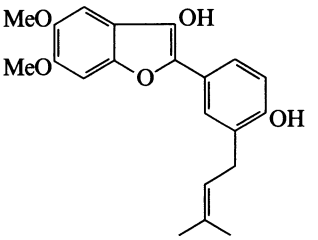
$C_{20}H_{20}O_4$ M 324.376
Constit. of *Nectandra glabrescens*. Cryst. (MeOH). Mp 83-85°.

Barbosa-Filho, J.M. *et al*, *Phytochemistry*, 1989, **28**, 1991.

Licobenzofuran L-80027

2-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-5,6-dimethoxy-3- benzofuranol, 9CI. 3-Hydroxy-2-(4-hydroxy-3-C-prenylphenyl)-5,6-dimethoxybenzofuran

[82209-75-4]



$C_{21}H_{22}O_5$ M 354.402
Isol. from *Glycyrrhiza* sp. Shows antibacterial props.

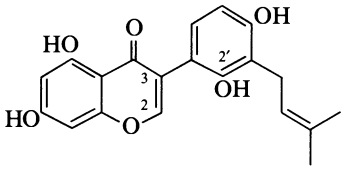
Chang, X. *et al*, *Zhongcaoyao*, 1981, **12**, 530; *CA*, **97**, 20701k.

Licoisoflavone A L-80028

Updated Entry replacing L-40024

[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. 3′-Isopentenyl-2′,4′,5,7-tetrahydroxyisoflavone. 2′,4′,5,7-Tetrahydroxy-3-C-prenylisoflavone. Phaseoluteone

[66056-19-7]



$C_{20}H_{18}O_6$ M 354.359

Constit. of the root of *Glycyrrhiza* spp., also from *Hardenbergia violacea* and *Phaseolus vulgaris*. Pale-yellow prisms (MeOH aq.).

Tetra-Ac: Mp 136-138°.

2,3-Dihydro, 2′-Me ether: [69573-59-7]. ***Sophoraisoflavanone A***

$C_{21}H_{22}O_6$ M 370.401

Isol. from aerial parts of *Sophora tomentosa*. Shows antifungal activity. Needles. Mp 178-180°. $[\alpha]_D^{22}$ −17.3° (EtOH).

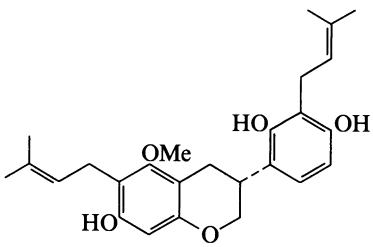
Kinoshita, T. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 141 (*isol, struct*)
Komatsu, M. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 3863 (*Sophoraisoflavanone A*)
Woodward, M.D., *Phytochemistry*, 1979, **18**, 363 (*isol, uv, pmr, ir*)
Tsukayama, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 136 (*synth*)

Licoricidin L-80029

Updated Entry replacing L-60025

2′,4′,7-Trihydroxy-5-methoxy-3′,6-diprenylisoflavan

[30508-27-1]



$C_{26}H_{32}O_5$ M 424.536

Struct. revised in 1988 (Me group previously considered to be at 7-posn.).

(R)-form

Constit. of *Glycyrrhiza glabra* and *G. uralensis*. Cryst. ($CHCl_3/Et_2O$). Mp 154-156°. $[\alpha]_D^{22.5}$ +20° (c, 1 in MeOH).

7-Me ether:

$C_{27}H_{34}O_5$ M 438.563

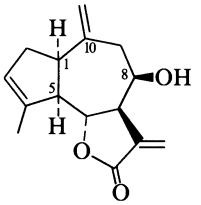
Constit. of *G. uralensis*. Called '5-*O*-Methyllicoricidin'.

Shibata, S. *et al*, *Chem. Pharm. Bull.*, 1968, **16**, 1932 (*isol*)
Kinoshita, T. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 141 (*isol*)
Shih, T.L. *et al*, *J. Org. Chem.*, 1987, **52**, 2029 (*synth*)
Fukai, T. *et al*, *Heterocycles*, 1988, **27**, 2309 (*isol, struct, cmr*)

Ligustrin L-80030

Updated Entry replacing L-50046

[21677-87-2]



$C_{15}H_{18}O_3$ M 246.305

Constit. of *Eupatorium ligustrinum* and of *Eriophyllum staechadifolium*. Cryst. (Me_2CO/Et_2O). Mp 135-137°. $[\alpha]_D$ +56°.

8-(2-Hydroxymethyl-4-hydroxy-2E-butenoyl): Constit. of *Stevia setifera*. Oil. $[\alpha]_D^{24}$ +4.9° (c, 0.7 in $CHCl_3$).

8-O-(4-Hydroxytigloyl): [100045-33-8].

$C_{20}H_{24}O_5$ M 344.407

Constit. of *Stevia mercedensis*. Oil.

8-O-(2,5-Dihydro-5-hydroxy-3-furancarboxylate): [100045-34-9].

$C_{20}H_{22}O_6$ M 358.390

Constit. of *S. mercedensis*. Oil. Mixt. of 5′-Epimers.

$\Delta^{1(10)}$-Isomer, 8-O-(2,5-dihydro-5-hydroxy-3-furancarboxylate): [100045-37-2].

$C_{20}H_{22}O_6$ M 358.390

Constit. of *S. mercedensis*. Oil. Mixt. of 5′-epimers.

8-Epimer: ***Epiligustrin***

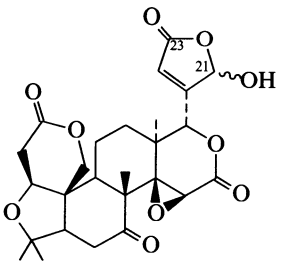
$C_{15}H_{18}O_3$ M 246.305

Constit. of *Leucanthemopsis pulverulenta*. Cryst. (Et_2O). Mp 132°. $[\alpha]_D$ +77.4° (c, 0.9 in $CHCl_3$). Not interrelated with Ligustrin.

[100045-35-0, 100045-38-3]

Romo, J. *et al*, *Tetrahedron*, 1968, **24**, 6087 (*isol*)
Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 673 (*isol*)
Bohlmann, F. *et al*, *Phytochemistry*, 1981, **20**, 2239 (*isol, stereochem*)
Ito, K. *et al*, *Phytochemistry*, 1982, **21**, 715 (*synth, pmr, epimer*)
De Pascual Teresa, J. *et al*, *Phytochemistry*, 1984, **23**, 1178 (*epimer*)
Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1986, 799 (*derivs*)

Limonexic acid L-80031



$C_{26}H_{30}O_{10}$ M 502.517

Constit. of *Phellodendron amurense*. Mp 285-286° dec. $[\alpha]_D^{25}$ −127.0°.

21-Oxo, 23ξ-alcohol: ***Isolimonexic acid***

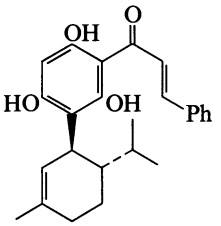
$C_{26}H_{30}O_{10}$ M 502.517

Constit. of *Tetradium glabrifolium*. Needles (EtOAc). Mp 295°. $[\alpha]_D$ −65° (c, 0.13 in MeOH). There is an error in the structure diagrams of the reference.

Kondo, Y. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1985, **105**, 742 (*Limonexic acid*)
Ng, K.M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1987, **50**, 1160 (*Isolimonexic acid*)

Linderachalcone L-80032

[120948-04-1]



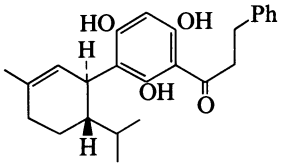
$C_{25}H_{28}O_4$ M 392.494
Constit. of *Lindera umbellata*. Yellow oil. $[\alpha]_D$ +17.8° (c, 0.4 in $CHCl_3$).

Ichino, K., *Phytochemistry*, 1989, **28**, 955.

Linderatin L-80033

Updated Entry replacing L-50048

[94530-80-0]



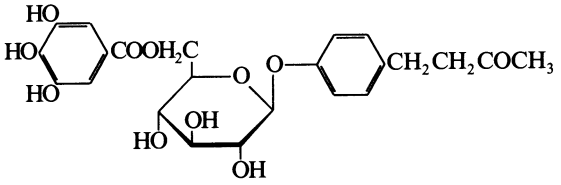
$C_{25}H_{30}O_4$ M 394.510
Constit. of leaves of *Lindera umbellata* var. *lancea*. Oil. $[\alpha]_D$ +19.1° (c, 0.45 in $CHCl_3$).

4′-Me ether: ***Methyllinderatin***
$C_{26}H_{32}O_4$ M 408.536
Constit. of *L. umbellata*. Oil. $[\alpha]_D$ +41.0° (c, 0.4 in $CHCl_3$).

Tanaka, H. *et al*, *Chem. Pharm. Bull.*, 1984, **32**, 3747 (*isol, struct*)
Ichino, K., *Phytochemistry*, 1989, **28**, 955 (*deriv*)

Lindleyin L-80034

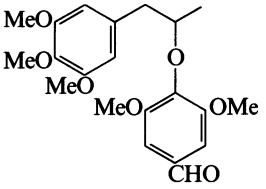
[59282-56-3]



$C_{23}H_{26}O_{11}$ M 478.452
Constit. of *Aeonium lindleyi*. Mp 210-211°. $[\alpha]_D$ +14° (c, 0.38 in Py).

González, A.G. *et al*, *Phytochemistry*, 1976, **15**, 344 (*isol, ir, uv, ms, struct*)

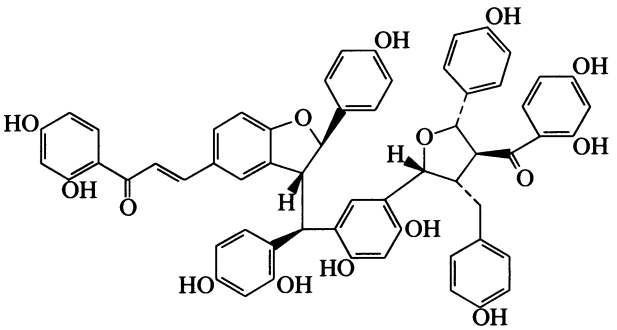
Liriolignal L-80035



$C_{21}H_{26}O_7$ M 390.432
Constit. of *Liriodendron tulipifera*. Oil. $[\alpha]_D^{25}$ +10.6° (c, 0.01 in $CHCl_3$).

Muhammad, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1177 (*isol, pmr, cmr*)

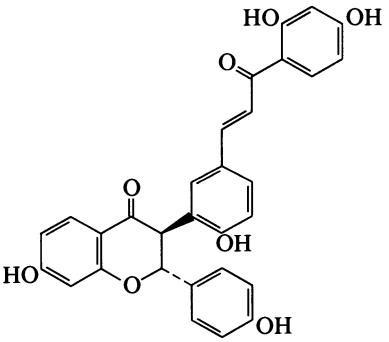
Lophirochalcone L-80036



$C_{60}H_{48}O_{15}$ M 1009.030
Constit. of *Lophira lanceolata*. Amorph. brown solid. $[\alpha]_D^{25}$ +181° (c, 0.6 in Me_2CO).

Tih, R.G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1807.

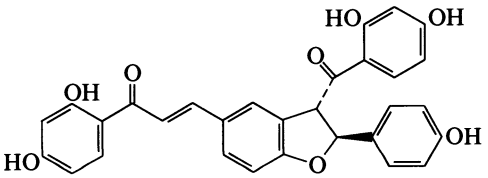
Lophirone B L-80037



$C_{30}H_{22}O_8$ M 510.499
Constit. of *Lophira lanceolata*. Yellow cryst. (Me_2CO). Mp 251-253° dec. $[\alpha]_D^{25}$ +7° (c, 0.4 in Me_2CO).

Ghogoma, R. *et al*, *Phytochemistry*, 1989, **28**, 1557.

Lophirone C L-80038

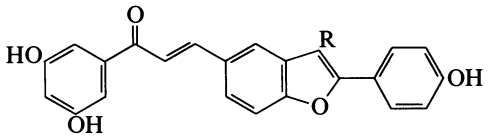


$C_{30}H_{22}O_8$ M 510.499
Constit. of *Lophira lanceolata*. Yellow cryst. (Me_2CO). Mp 191-193° dec. $[\alpha]_D^{25}$ −16.3° (c, 0.5 in Me_2CO).

Ghogoma, R. *et al*, *Phytochemistry*, 1989, **28**, 1557.

Lophirone D L-80039

[122127-70-2]



R = CHO

$C_{24}H_{16}O_6$ M 400.387
Constit. of *Lophira lanceolata*. Yellow cryst. (Me_2CO). Mp 270-276° dec.

Ghogomu, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 284 (*isol*, *pmr*, *cmr*)

Lophirone E L-80040

[122127-72-4]

As Lophirone D, L-80039 with

R = H

$C_{23}H_{16}O_5$ M 372.376
Constit. of *Lophira lanceolata*. Yellow cryst. (Me_2CO). Mp 266-268°.

Ghogomu, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 284 (*isol*, *pmr*, *cmr*)

20(29)-Lupene-3,16-diol L-80041

$C_{30}H_{50}O_2$ M 442.724

(3β,16β)-form
Isol. from leaves of *Beyera leschenaultii*. Needles (Me_2CO). Mp 218-219°. $[\alpha]_D$ +23° (c, 1.18 in $CHCl_3$).

Baddeley, G.V. *et al*, *Aust. J. Chem.*, 1964, **17**, 908.

20(29)-Lupene-3,24-diol L-80042

$C_{30}H_{50}O_2$ M 442.724

3β-form [119285-48-2]
Constit. of *Phyllanthus flexuosus*. Needles ($MeOH/CHCl_3$). Mp 249-250°. $[\alpha]_D^{23}$ +40.5° (c, 0.58 in $CHCl_3$).

Tanaka, R. *et al*, *Phytochemistry*, 1988, **27**, 3563.

20(29)-Lupen-7-ol L-80043

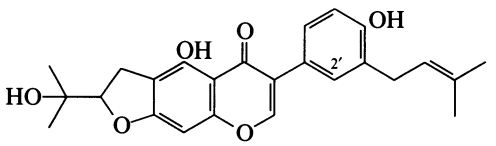
$C_{30}H_{50}O$ M 426.724

7β-form [123617-37-8]
Constit. of *Psoralea plicata*. Cryst. (C_6H_6/MeOH). Mp 192°. $[\alpha]_D$ +19° (c, 0.3 in $CHCl_3$).

Rasool, N. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 749 (*isol*, *pmr*, *cmr*)

Lupinisoflavone G L-80044

[121747-91-9]



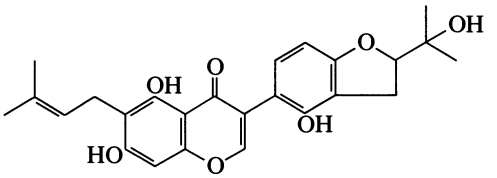
$C_{25}H_{26}O_6$ M 422.477
Constit. of *Lupinus albus*. Gum.

2′-Hydroxy: [121747-92-0]. ***Lupinisoflavone H***
$C_{25}H_{26}O_7$ M 438.476
Constit. of *L. albus*. Amorph. powder.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Lupinisoflavone I L-80045

[121768-55-6]

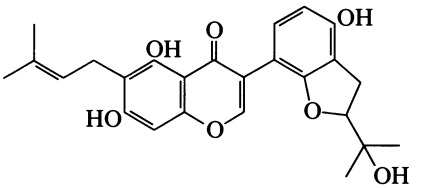


$C_{25}H_{26}O_7$ M 438.476
Constit. of *Lupinus albus*. Amorph. powder.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Lupinisoflavone J L-80046

[121747-95-3]

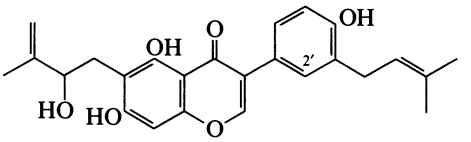


$C_{25}H_{26}O_7$ M 438.476
Constit. of *Lupinus albus*. Amorph. powder.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Lupinisol A L-80047

[121747-99-7]



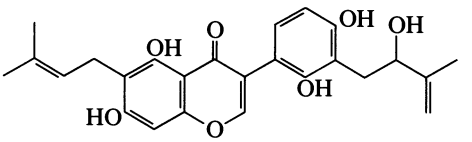
$C_{25}H_{26}O_6$ M 422.477
Constit. of *Lupinus albus*. Gum.

2′-Hydroxy: [121748-00-3]. ***Lupinisol B***
$C_{25}H_{26}O_7$ M 438.476
Constit. of *L. albus*. Gum.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Lupinisol C L-80048

[121748-01-4]

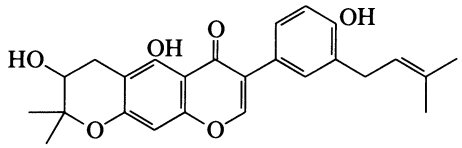


$C_{25}H_{26}O_7$ M 438.476
Constit. of *Lupinus albus*. Gum.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Lupinisolone A L-80049

[121747-96-4]

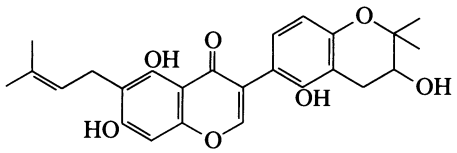


$C_{25}H_{26}O_6$ M 422.477
Constit. of *Lupinus albus*. Gum.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Lupinisolone B L-80050

[121747-97-5]

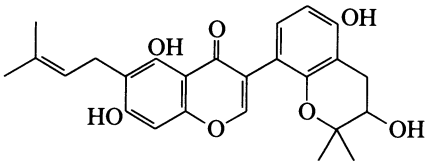


$C_{25}H_{26}O_7$ M 438.476
Constit. of *Lupinus albus*. Gum.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Lupinisolone C L-80051

[121747-98-6]



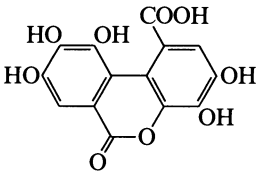
$C_{25}H_{26}O_7$ M 438.476
Constit. of *Lupinus albus*. Glassy solid.

Tahara, S. *et al*, *Phytochemistry*, 1989, **28**, 901.

Luteolic acid L-80052

*3,4,8,9,10-Pentahydroxy-6-oxo-6*H*-dibenzo*[b,d]*pyran-1-carboxylic acid, 9CI*

[476-67-5]



$C_{14}H_8O_9$ M 320.212
Isol. from fruits of *Terminalia chebula*. Reddish needles (AcOH). Mp 338-342° dec.

Diglucoside:
$C_{26}H_{28}O_{19}$ M 644.496
Isol. from leaf tannin of *Lagerstroemia subcostata*. $[\alpha]_D^{20}$ +40.8° (c, 1 in H_2O). Exact struct. unknown.

Nierenstein, M., *Ber.*, 1908, **41**, 3015; 1909, **42**, 353.
Ishii, M., *CA*, 1951, **45**, 2698 (*glucoside*)

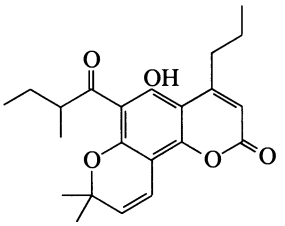
M

MAB 6 — M-80001

Updated Entry replacing M-00009

5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-propyl-2H,8H-benzo[1,2-b:3,4-b′]dipyran-2-one

[30390-19-3]



$C_{22}H_{26}O_5$ M 370.444

Constit. of *Mammea africana*. Gum. λ_{max} 227 (log ϵ 4.25), 285(4.20) and 330 nm (3.72) (0.1N HCl).

Analogue (1): [34107-36-3]. ***5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-propyl-2H,8H-benzo[1,2-b, 3,4-b′]dipyran-2-one, 9CI***

$C_{21}H_{24}O_5$ M 356.418

Isol. from *M. americana*. Has 2-Methyl-1-oxopropyl in place of the 2-methyl-1-oxobutyl residue.

Analogue (2): [34107-35-2]. ***5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-propyl-2H,8H-benzo[1,2-b:3,4-b′]dipyran-2-one, 9CI***

$C_{21}H_{24}O_5$ M 356.418

Isol. from *M. americana*. Has 1-oxobutyl in place of 2-methyl-1-oxobutyl.

Analogue (3): [39036-48-1]. ***5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-pentyl-2H,8H-benzo[1,2-b:3,4-b′]dipyran-2-one, 9CI***

$C_{24}H_{30}O_5$ M 398.498

Isol. from *M. americana*. Has *n*-pentyl in place of the *n*-propyl residue.

Analogue (4): [34124-91-9]. ***5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-propyl-2H,8H-benzo[1,2-b:3,4-b′]dipyran-2-one, 9CI***

$C_{22}H_{26}O_5$ M 370.444

Isol. from *M. americana* and *M. africana*. Has 3-methyl-1-oxobutyl in place of 2-methyl-1-oxobutyl.

Analogue (5): [39036-47-0]. ***5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-pentyl-2H,8H-benzo[1,2-b:3,4-b′]dipyran-2-one, 9CI***

$C_{24}H_{30}O_5$ M 398.498

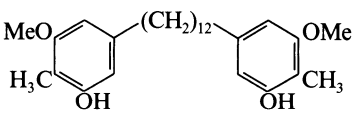
Isol. from *M. americana*. Has *n*-butyl in place of propyl and 3-methyl-1-oxobutyl in place of 2-methyl-1-oxobutyl.

Carpenter, I. *et al*, *J. Chem. Soc. C*, 1971, 3783 (*isol, struct*)
Games, D.E., *Tetrahedron Lett.*, 1972, 3187 (*analogues*)

Maesol — M-80002

3,3′-(1,2-Dodecanediyl)bis[5-methoxy-6-methylphenol], 9CI.
1,12-Bis(3-hydroxy-5-methoxy-4-methylphenyl)dodecane

[119766-98-2]



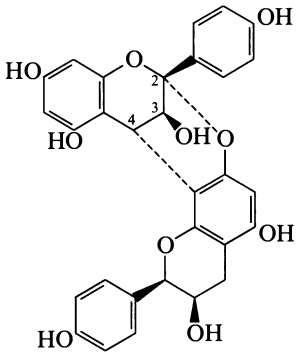
$C_{28}H_{42}O_4$ M 442.637

Constit. of *Maesa montana* and *M. indica*. Cryst. Mp 76-78°.

Wall, M.E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1227 (*isol, pmr, cmr*)

Mahuannin A — M-80003

[82765-89-7]



Absolute configuration

$C_{30}H_{24}O_{10}$ M 544.514

Constit. of *Ephedra* spp. Amorph. powder.

2,3,4-Triepimer: [82796-37-0]. ***Mahuannin B***

$C_{30}H_{24}O_{10}$ M 544.514

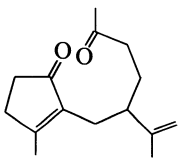
Constit. of *E.* spp. Amorph. powder.

Hikino, H. *et al*, *Heterocycles*, 1982, **19**, 1381.

Mandassidione — M-80004

3-Methyl-2-[2-(1-methylethenyl)-5-oxohexyl]-2-cyclopenten-1-one, 9CI

[118855-38-2]



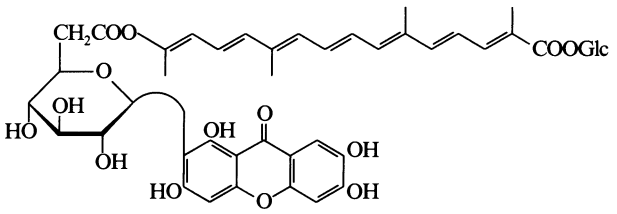
$C_{15}H_{22}O_2$ M 234.338

Constit. of *Cyperus articulatus*. Oil. $[\alpha]_D^{25}$ −9.10° (c, 0.74 in $CHCl_3$). A cleaved guaiane.

Nyasse, B. *et al*, *Phytochemistry*, 1988, **27**, 3319.

Mangicrocin M-80005

[122575-51-3]

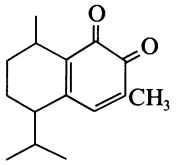


$C_{45}H_{50}O_{19}$ M 894.879
Constit. of saffron. $[\alpha]_D^{28}$ +17.5° (c, 0.53 in MeOH).

Ghosal, S. *et al*, *J. Chem. Res.* (*S*), 1989, 70.

Mansonone A M-80006

Updated Entry replacing M-00135
5,6,7,8-Tetrahydro-3,8-dimethyl-5-(1-methylethyl)-1,2-naphthalenedione, 9CI
[7715-94-8]

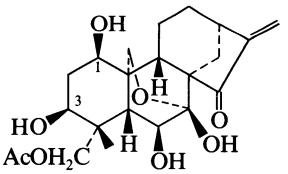


$C_{15}H_{20}O_2$ M 232.322
Constit. of *Mansonia altissima* heartwood. Red cryst. (cyclohexane). Mp 117-118°. $[\alpha]_D$ +680° (c, 0.2 in $CHCl_3$). λ_{max} 209 (log ϵ 4.32) and 430 nm (2.93) (EtOH).

Marini Bettolo, G.B. *et al*, *Tetrahedron Lett.*, 1965, 4857 (*isol*, *uv*, *pmr*)
Tanaka, N. *et al*, *Tetrahedron Lett.*, 1966, 2767 (*isol*, *uv*)
Dumas, M.T. *et al*, *Experientia*, 1983, **39**, 1089 (*isol*)
Murali, D. *et al*, *Indian J. Chem.*, *Sect. B*, 1987, **26**, 668 (*synth*)

Maoecrystal I M-80007

ent-*19-Acetoxy-7β,20-epoxy-1α,3α,6α,7α-tetrahydroxy-16-kauren-15-one*

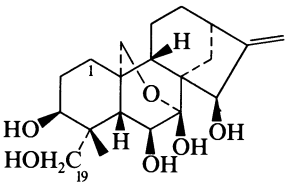


$C_{22}H_{30}O_8$ M 422.474
Constit. of *Rabdosia eriocalyx*. Cryst. (Me_2CO/hexane). Mp 205-206°.

1-Deoxy, 3-Ac: ***Maeocrystal* J**
$C_{24}H_{32}O_8$ M 448.512
Constit. of *R. eriocalyx*. Cryst. (Me_2CO/hexane). Mp 249-250°. $[\alpha]_D$ −49.7° (c, 1 in MeOH).

Shen, X. *et al*, *Phytochemistry*, 1989, **28**, 855.

Maoecrystal K M-80008



$C_{20}H_{30}O_6$ M 366.453
Constit. of *Rabdosia eriocalyx*. Cryst. Mp 191.5-193°. $[\alpha]_D^{26.5}$ −1.3° (c, 1 in MeOH).

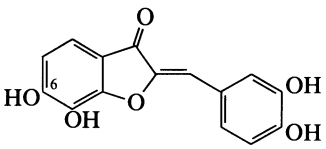
19-O-β-D-Glucopyranoside: ***Rabdoside 1***
$C_{26}H_{40}O_{11}$ M 528.595
Constit. of *R. eriocalyx*. Cryst. Mp 179-180°. $[\alpha]_D^{26.5}$ −4.6° (c, 1 in MeOH).

1β-Hydroxy-19-O-β-D-glucopyranoside: ***Rabdoside 2***
$C_{26}H_{40}O_{12}$ M 544.595
Constit. of *R. eriocalyx*. Cryst. Mp 170-171°. $[\alpha]_D^{26.5}$ −4.5° (c, 1 in MeOH).

Isogai, A. *et al*, *Phytochemistry*, 1989, **28**, 2427 (*isol*, *pmr*, *cmr*)

Maritimetin M-80009

Updated Entry replacing D-04380
6,7-Dihydroxy-2-(3′,4′-dihydroxyphenylmethylene)-3(2H)-benzofuranone, 9CI. 3′,4′,6,7-Tetrahydroxyaurone
[576-02-3]



$C_{15}H_{10}O_6$ M 286.240
Isol. from flowers of *Coreopsis maritima*, *C. gigantea*, *C. tinctoria* and *Baeria chrysostoma*. Used in flavouring. Orange needles (H_2O). Mp 292° dec.

Tetra-Ac: Cryst. (EtOH). Mp 190-192°.

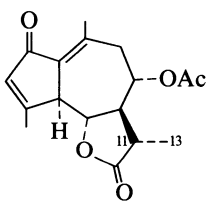
Tetra-Me ether: Yellow needles (EtOH aq.). Mp 156-157°.

6-O-β-D-Glucopyranoside: [490-54-0]. ***Maritimein***
$C_{21}H_{20}O_{11}$ M 448.382
Pigment present in the flowers of *Coreopis maritima*, *C. tinctoria* and *Baeria chrysotoma*. Yellow cryst (EtOAc). Mp 208-214°.

Harborne, J.B. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 825, 829 (*isol*, *struct*)
Shimokoriyama, M. *et al*, *J. Org. Chem.*, 1960, **25**, 1956 (*isol*)
Farkas, L. *et al*, *Chem. Ber.*, 1965, **98**, 2103 (*synth*)
Huke, M. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1969, **302**, 401 (*synth*)

Matricarin M-80010

Updated Entry replacing M-00188
Artilesin A
[5989-43-5]



$C_{17}H_{20}O_5$ M 304.342

Constit. of *Artemisia* spp. Also from *Matricaria chamomilla* and *Achillea lanulosa*. Cryst. (C_6H_6/pet. ether). Mp 193-195°. $[\alpha]_D^{23}$ +23.5° (c, 0.65 in $CHCl_3$).

O-*De-Ac:* ***Austrisin.*** *Desacetylmatricarin*
$C_{15}H_{18}O_4$ M 262.305
Isol. from *Artemisia tilesii*, *A. austriaca*, *A. leucodes*, *A. juncea* and *Achillea lanulosa*. Cryst. + $1H_2O$ (C_6H_6/Me_2CO). Mp 123-125°, Mp 143-146° (double Mp, hydrate).

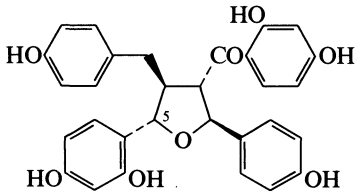
Deacetoxy: ***Leucomisin.*** *Leucodin. Desacetoxymatricarin*
$C_{15}H_{18}O_3$ M 246.305
Isol. from *Artemisia leucodes*. Prisms (EtOH). Mp 202-203°. $[\alpha]_D^{20}$ +55.9° (c, 2.86 in $CHCl_3$).

11,13-Didehydro: [69904-98-9]. ***11,13-Dehydromatricarin***
$C_{17}H_{18}O_5$ M 302.326
Constit. of *Anthanasia* and *Pentzia* spp. Cryst. (Et_2O/pet. ether). Mp 146°. $[\alpha]_D^{24}$ +120.8° (c, 1 in $CHCl_3$).

Herz, W. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 1139 (*isol*)
Rybalko, K.S., *Zh. Obshch. Khim.*, 1963, **33**, 2734 (*Leucomisin*)
White, E.H. *et al*, *Tetrahedron*, 1969, **25**, 2099 (*struct*)
Bohlmann, F. *et al*, *Phytochemistry*, 1978, **17**, 1595 (*isol*)
Martinez, V. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 211 (*pmr, cmr*)

Mbamichalcone M-80011

Updated Entry replacing M-70014
[119264-65-2]



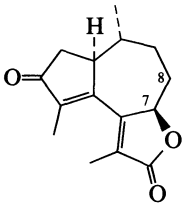
Relative configuration

$C_{30}H_{26}O_8$ M 514.531
Constit. of *Lophira alata*. Amorph. solid. $[\alpha]_D^{25}$ −47.8° (c, 0.65 in MeOH).

5-Epimer: [122621-92-5]. ***Isombamichalcone***
$C_{30}H_{26}O_8$ M 514.531
Constit. of bark of *L. lanceolata*. Amorph. powder. $[\alpha]_D^{20}$ −129° (c, 0.5 in Me_2CO). Abs. config. not detd.

Tih, A.E. *et al*, *Tetrahedron Lett.*, 1988, **29**, 5797 (*struct*)
Tih, R.G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1807 (*Isombamichalcone*)

Melicophyllone A M-80012



$C_{15}H_{18}O_3$ M 246.305
Constit. of *Melicope triphylla*. Plates. Mp 106-107°. $[\alpha]_D$ −371° ($CHCl_3$).

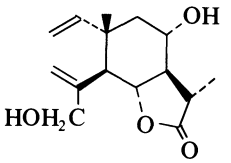
7-Hydroxy: ***Melicophyllone B***
$C_{15}H_{18}O_4$ M 262.305
Constit. of *M. triphylla*. Needles. Mp 171-172°. $[\alpha]_D$ −38° ($CHCl_3$).

7α,8β-Dihydroxy: ***Melicophyllone C***
$C_{15}H_{18}O_5$ M 278.304
Constit. of *M. triphylla*. Needles. Mp 254°. $[\alpha]_D$ −56.23° (Me_2CO).

Wu, T.-S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 956 (*cryst struct*)
Jong, T.-T. *et al*, *J. Chem. Res.* (*S*), 1989, 273; *J. Chem. Res.* (*M*), 1701 (*isol*)

Melitensin M-80013

Updated Entry replacing M-00281
8α,15-Dihydroxy-1,3-elemadien-12,6α-olide
[38049-38-6]



$C_{15}H_{22}O_4$ M 266.336
Constit. of *Centaurea melitensis* and *C. aspera* var. *stenophylla*. Cryst. Mp 167-168°. $[\alpha]_D$ +85°.

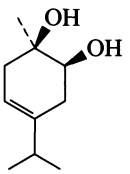
11,13-Didehydro: ***Dehydromelitensin***
$C_{15}H_{20}O_4$ M 264.321
Constit. of *Onopordon corymbosum*. Oil.

11,13-Didehydro, 8-(2-hydroxymethyl-2-propenoyl): ***Dehydromelitensin 4-hydroxymethacrylate***
$C_{19}H_{24}O_6$ M 348.395
Constit. of *O. corymbosum*. Oil.

González, A.G. *et al*, *An. Quim.*, 1971, **67**, 1243; 1974, **70**, 158 (*isol, struct, synth*)
Tortajada, A. *et al*, *Phytochemistry*, 1988, **27**, 3549 (*cryst struct*)
Cardona, Ma.L. *et al*, *Phytochemistry*, 1989, **28**, 1264 (*deriv*)

p-Menth-4-ene-1,2-diol M-80014

1-Methyl-4-(1-methylethyl)-4-cyclohexene-1,2-diol, 9CI. 4-Isopropyl-1-methyl-4-cyclohexene-1,2-diol
[4031-37-2]

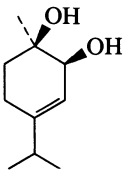


$C_{10}H_{18}O_2$ M 170.251
Constit. of *Ferula jaeschkeana*. Oil.
[21473-37-0, 94492-01-0]

Kapahi, B.K. *et al*, *Pafai*, 1985, **7**, 23.

p-Menth-3-ene-1,2-diol M-80015

4-Isopropyl-1-methyl-3-cyclohexene-1,2-diol

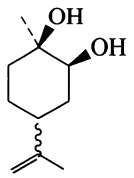


$C_{10}H_{18}O_2$ M 170.251
Constit. of *Ferula jaeschkeana*. Oil.

Kapahi, B.K. *et al*, *Pafai*, 1985, **7**, 23.

p-Menth-7-ene-1,2-diol M-80016

4-Isopropenyl-1-methyl-1,2-cyclohexanediol



$C_{10}H_{18}O_2$ M 170.251
Constit. of *Ferula jaeschkeana*. Oil.

Kapahi, B.K. *et al*, *Pafai*, 1985, **7**, 23; *CA*, **103**, 92620y.

Mercaptoacetaldehyde M-80017

Updated Entry replacing M-50049
[4124-63-4]

$HSCH_2CHO$

C_2H_4OS M 76.119
Known only in soln. Readily dimerises

Di-Et acetal: [53608-94-9]. *2,2-Diethoxyethanethiol, 9CI. Mercaptoacetal*
$C_6H_{14}O_2S$ M 150.241
Liq. with acetal odour. $Bp_{0.3}$ 81°, $Bp_{0.12}$ 59-60°. n_D^{25} 1.4391. Dec. slowly on standing.

S-*Me:* (*Methylthio*)*acetaldehyde*
C_3H_6OS M 90.146
Bp 129-134°, Bp_{10} 35°.

S-*Me, 2,4-dinitrophenylhydrazone:* Cryst. (EtOH aq.). Mp 131.0-131.5°.

S-*Me, semicarbazone:* Mp 133.5-134°.

S-*Me, di-Me acetal:* [40015-15-4]. *1,1-Dimethoxy-2(methylthio)ethane, 9CI*
$C_5H_{12}O_2S$ M 136.215
Bp_{10} 55°.

S-*Et:* [33672-79-6]. (*Ethylthio*)*acetaldehyde*
C_4H_8OS M 104.173
Bp_{10} 46.5°.

S-*Et, 2,4-dinitrophenylhydrazone:* Mp 125.5-126°.

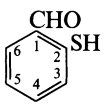
S-*Et, semicarbazone:* Mp 93-93.5°.

S-*Me, di-Et acetal:* [51517-03-4]. *2-(Ethylthio)-1,1-dimethoxyethane, 9CI*
$C_6H_{14}O_2S$ M 150.241
Bp_{11} 63-64°.

Hesse, G. *et al*, *Chem. Ber.*, 1952, **85**, 924, 933.
Wick, E.H. *et al*, *J. Agric. Food Chem.*, 1961, **9**, 289 (*deriv, synth*)
Org. Synth., Coll. Vol., 4, 1963, 295.
Gassman, P.G. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 5495 (*deriv, synth*)
Mikolajczyk, M. *et al*, *Synthesis*, 1987, 659 (*synth, pmr, ms, bibl*)

2-Mercaptobenzaldehyde M-80018

2-Formylbenzenethiol
[29199-11-9]



C_7H_6OS M 138.190
Yellow oil.

Me ether: [7022-45-9]. *2-(Methylthio)benzaldehyde*
C_8H_8OS M 152.217
Pale yellow oil. Bp_{19} 149-150°.

Me ether, 2,4-dinitrophenylhydrazone: [52369-78-5]. Mp 243°.

Eistert, B. *et al*, *Chem. Ber.*, 1964, **97**, 1470 (*synth, deriv*)
Ohno, S. *et al*, *Chem. Pharm. Bull.*, 1986, **34**, 1589 (*synth, deriv, pmr*)
Kasmai, H.S. *et al*, *Synthesis*, 1989, 763 (*synth, deriv, pmr, bibl*)

3-Mercaptobenzaldehyde M-80019

3-Formylbenzenethiol
C_7H_6OS M 138.190

Me ether: [73771-35-4]. *3-(Methylthio)benzaldehyde*
Oil. $Bp_{0.05}$ 82-83°.

Eurby, M. *et al*, *Synth. Commun.*, 1981, **11**, 849 (*synth, pmr, ms*)

4-Mercaptobenzaldehyde M-80020

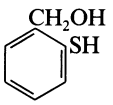
4-Formylbenzenethiol
[91358-96-2]
C_7H_6OS M 138.190
Oil.

Me ether: [3446-89-7]. *4-(Methylthio)benzaldehyde*
C_8H_8OS M 152.217
Pale yellow oil. Bp 273°, Bp_1 101-103°.

Friedländer, P. *et al*, *Chem. Ber.*, 1912, **45**, 2083 (*synth*)
Rivett, D.E., *Aust. J. Chem.*, 1979, **32**, 1601 (*synth, deriv*)
Young, R.N. *et al*, *Tetrahedron Lett.*, 1984, **25**, 1753 (*synth*)
Creary, X. *et al*, *J. Org. Chem.*, 1986, **57**, 1110 (*synth, deriv, pmr*)

2-Mercaptobenzenemethanol, 9CI M-80021

2-Mercaptobenzyl alcohol. 2-(Hydroxymethyl)thiophenol
[4521-31-7]



C_7H_8OS M 140.206
Needles (pentane). Mp 31-32°.

S-*Me:* [33384-77-9].
$C_8H_{10}OS$ M 154.232
$Bp_{0.001}$ 88°.

S-Benzyl:
$C_{14}H_{14}OS$ M 230.330
Needles (pet. ether). Mp 48.5-49.5°.

Disulfide:
$C_{14}H_{14}O_2S_2$ M 278.395
Cryst. Mp 141-142°.

Grice, R. *et al*, *J. Chem. Soc.*, 1963, 1947 (*deriv*)
Stacy, G.W. *et al*, *J. Org. Chem.*, 1965, **30**, 4074 (*synth, ir*)
Arnoldi, A. *et al*, *Synthesis*, 1988, 155 (*synth*)

3-Mercaptobenzenemethanol M-80022

3-Mercaptobenzyl alcohol. 3-(Hydroxymethyl)thiophenol
[83794-86-9]
C_7H_8OS M 140.206
$Bp_{0.001}$ 88°.

S-Me: [59083-33-9].
$C_8H_{10}OS$ M 154.232
$Bp_{0.001}$ 98°.

Disulfide:
$C_{14}H_{14}O_2S_2$ M 278.395
Prisms (Et_2O/pet. ether).

Grice, R. *et al*, *J. Chem. Soc.*, 1963, 1947 (*synth*)
Thurber, T.C. *et al*, *J. Heterocycl. Chem.*, 1982, **19**, 961 (*synth, pmr*)

4-Mercaptobenzenemethanol M-80023

4-Mercaptobenzyl alcohol. 4-(Hydroxymethyl)thiophenol

[53339-53-0]

C_7H_8OS M 140.206

Plates (CCl_4/pet. ether). Mp 52-54°.

S-*Me:* [3446-90-0].

$C_8H_{10}OS$ M 154.232

Cryst. Mp 37-39°. $Bp_{0.01}$ 100°.

Disulfide:

$C_{14}H_{14}O_2S_2$ M 278.395

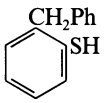
Needles (Me_2CO aq.). Mp 130-132°.

Grice, R. *et al*, *J. Chem. Soc.*, 1963, 1947 (*synth*)

2-Mercaptodiphenylmethane M-80024

2-(Phenylmethyl)benzenethiol, 9CI. 2-Benzylbenzenethiol. 1-Benzyl-2-mercaptobenzene

[120454-34-4]



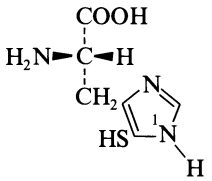
$C_{13}H_{12}S$ M 200.304

Pale brown solid (pet. ether). Mp 44-47°.

Cadogan, J.I.G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2875 (*synth, pmr, cmr, ms*)

5-Mercaptohistidine, 9CI M-80025

5-Thiolhistidine



$C_6H_9N_3O_2S$ M 187.222

(S)-form

L-form

1-Me: [62982-24-5]. ***5-Mercapto-1-methylhistidine***

$C_7H_{11}N_3O_2S$ M 201.249

Constit. of the unfertilised eggs of the sea urchin *Paracentrotus lividus*. Also a component of the struct. of adrenochrome, an Fe(III) contg. peptide from *Octopus vulgaris*.

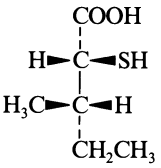
1-Me, disulfide: [83471-81-2]. ***5,5′-Dithiobis[1-methylhistidine]*, 9CI**

$C_{14}H_{20}N_6O_4S_2$ M 400.482

Isol. from the unfertilised eggs of *P. lividus*. Prisms (EtOH aq.). Mp 202-205° (darkens). $[\alpha]_D^{20}$ +76° (c, 1.2 in 0.1*M* HCl).

Palumbo, A. *et al*, *Tetrahedron Lett.*, 1982, **23**, 3207 (*isol, uv, pmr, cmr, struct, deriv*)

2-Mercapto-3-methylpentanoic acid M-80026



$C_6H_{12}O_2S$ M 148.226

(2R,3S)-form

$Bp_{0.02}$ 60°. $[\alpha]_D^{20}$ +10.3° (c, 2.4 in $CHCl_3$). Optically pure.

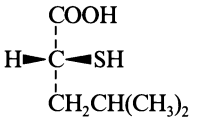
S-*Benzoyl:*

$C_{13}H_{16}O_3S$ M 252.334

Thick oil, solidifies on standing. Mp *ca* 35°. $[\alpha]_D^{20}$ +24.2° (c, 2 in C_6H_6).

Strijtreen, B. *et al*, *Tetrahedron*, 1987, **43**, 5039 (*synth, pmr, cmr*)

2-Mercapto-4-methylpentanoic acid M-80027



(*R*)-*form*

$C_6H_{12}O_2S$ M 148.226

(R)-form

$Bp_{0.01}$ 70°. $[\alpha]_D^{22}$ +25.1° (c, 11 in $CHCl_3$).

(S)-form [66386-08-1]

$[\alpha]_D^{20}$ −23.8° (c, 1.8 in Et_2O).

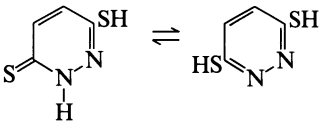
Yankeelov, J. *et al*, *J. Org. Chem.*, 1978, **43**, 1623 (*synth, abs config*)

Strijtveen, B. *et al*, *Tetrahedron*, 1987, **43**, 5039 (*synth, pmr, cmr*)

3-Mercapto-6(1*H*)-pyridazinethione M-80028

3,6-Dimercaptopyridazine. 1,2-Dihydro-3,6-pyridazinedithione, 9CI

[1445-58-5]



$C_4H_4N_2S_2$ M 144.221

Exists mainly in thione form. Mp >230° dec. Also reported with double Mp 190° and 246° dec.

S-*Ac:*

$C_6H_6N_2OS_2$ M 186.258

Mp 152-153°.

S,S-*Di-Ac:*

$C_8H_8N_2O_2S_2$ M 228.295

Mp 123-124°.

1,S-*Di-Me:* [54320-90-0]. *2-Methyl-6-(methylthio)-3(2*H*)-pyridazinethione, 9CI*

$C_6H_8N_2S_2$ M 172.275

Mp 86-87° (73-74°).

Di-S-*Me:* [37813-54-0]. *3,6-Bis(methylthio)pyridazine*

$C_6H_8N_2S_2$ M 172.275

Needles (hexane). Mp 125-126.5°.

Di-S-*Me; B,MeI:* Cryst. (MeOH/2-methyl-2-propanol). Mp 161-163°.

Druey, J. *et al*, *Helv. Chim. Acta*, 1954, **37**, 121 (*synth, deriv*)

Stanovnik, B. *et al*, *Croat. Chim. Acta*, 1964, **36**, 81 (*synth, tautom*)

Pollak, A. *et al*, *Can. J. Chem.*, 1966, **44**, 829 (*synth*)

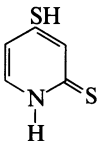
Barlin, G.B., *J. Chem. Soc., Perkin Trans.* 2, 1974, 1199 (*synth, deriv, tautom*)

Boger, D.L. *et al*, *J. Org. Chem.*, 1988, **53**, 1415 (*deriv, synth, pmr, ir, ms*)

4-Mercapto-2(1*H*)-pyridinethione, 9CI M-80029

2,4-Dimercaptopyridine. 2,4-Pyridinedithiol

[28508-52-3]



$C_5H_5NS_2$ M 143.233
Yellow solid. Mp 135-137°.

4-S-Me: [71506-84-8]. *4-(Methylthio)-2(1H)-pyridinethione*
$C_6H_7NS_2$ M 157.260
Yellow solid. Mp 220-223° (rapid htg.).

N,S-*Di-Me:* [71506-86-0]. *1-Methyl-4-(methylthio)-2(1H)-pyridinethione*
$C_7H_9NS_2$ M 171.287
Pale yellow solid. Mp 155-156°.

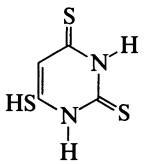
Di-S-Me: [71506-85-9]. *2,4-Bis(methylthio)pyridine*
$C_7H_9NS_2$ M 171.287
Bp_2 130°, $Bp_{0.05}$ 99°.

Di-S-Me, S-tetroxide: [62916-42-1]. *2,4-Bis(methylsulfonyl)pyridine*
$C_7H_9NO_4S_2$ M 235.284
Mp 167-168°.

Krowicki, K., *Pol. J. Chem.* (*Rocz. Chem.*), 1979, **53**, 701 (*synth, pmr, derivs*)
Woods, S.G. *et al*, *J. Heterocycl. Chem.*, 1984, **21**, 97 (*deriv*)

6-Mercapto-2,4(1*H*,3*H*)-pyrimidinedithione, 9CI — M-80030

2,4,6-Trithiobarbituric acid, 8CI. 2,4,6-Trimercaptopyrimidine
[6308-40-3]



$C_4H_4N_2S_3$ M 176.287
Several tautomers possible. Orange-yellow cryst. Mp >360°.

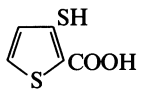
2-S-Me:
$C_5H_6N_2S_3$ M 190.314
Pale yellow cryst. Mp >360°.

[5658-04-8]

Koppel, H.C. *et al*, *J. Org. Chem.*, 1961, **26**, 792 (*synth*)
Netzel, D.A. *et al*, *Appl. Spectrosc.*, 1968, **22**, 170 (*ir*)
Hübsch, W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 744 (*synth*)

3-Mercapto-2-thiophenecarboxylic acid — M-80031

[90033-62-8]



$C_5H_4O_2S_2$ M 160.217
Solid (H_2O). Mp 152-153°.

Corral, C. *et al*, *Synthesis*, 1984, 172 (*synth*)
Corral, C. *et al*, *Org. Prep. Proced. Int.*, 1985, **17**, 163 (*synth, pmr*)

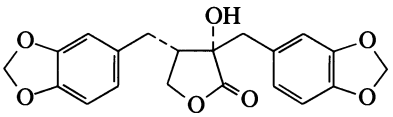
4-Mercapto-3-thiophenecarboxylic acid — M-80032

[98077-07-7]
$C_5H_4O_2S_2$ M 160.217
Cryst. (AcOH). Mp 215-216°.

Corral, C. *et al*, *Org. Prep. Proced. Int.*, 1985, **17**, 163 (*synth, pmr*)

Meridinol — M-80033

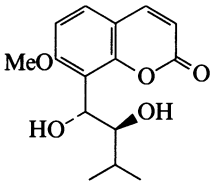
[120051-54-9]



$C_{20}H_{18}O_7$ M 370.358
Constit. of *Zanthoxylum fagara*. Needles(EtOAc/pet. ether). Mp 122-123°. $[\alpha]_D^{25}$ −30° (c, 0.1 in $CHCl_3$).

Amaro-Luis, J.M. *et al*, *Phytochemistry*, 1988, **27**, 3933 (*isol, cryst struct*)

Merrillin — M-80034

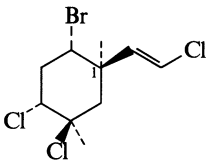


$C_{15}H_{18}O_5$ M 278.304
Constit. of *Merrillia caloxylon*. Plates. Mp 68°. $[\alpha]_D^{20}$ −15.6° (c, 0.135 in $CHCl_3$).

Zakaria, M.B. *et al*, *Phytochemistry*, 1989, **28**, 657.

Mertensene — M-80035

Updated Entry replacing B-30236
2-Bromo-4,5-dichloro-1-(2-chlorovinyl)-1,5-dimethylcyclohexane
[66389-40-0]

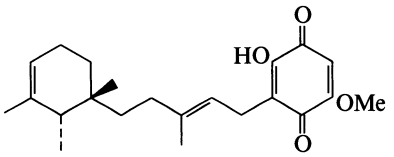


$C_{10}H_{14}BrCl_3$ M 320.483
Constit. of *Plocamium mertensii* and *P. hamatum*. Needles (hexane). Mp 105.5-106°. $[\alpha]_D$ +20° (c, 0.3 in $CHCl_3$).

1-Epimer: [95044-70-5]. ***Coccinene*†**
$C_{10}H_{14}BrCl_3$ M 320.483
Constit. of *P. coccineum*. Cryst. (hexane). Mp 65°. $[\alpha]_D^{25}$ −24° (c, 0.82 in $CHCl_3$).

Norton, R.S. *et al*, *Tetrahedron Lett.*, 1977, 3905 (*isol*)
Capon, R.J. *et al*, *Aust. J. Chem.*, 1984, **37**, 537 (*isol*)
Castedo, L. *et al*, *J. Nat. Prod.* (*Lloydia*), 1984, **47**, 724 (*isol, Coccinene*)
Crews, P. *et al*, *J. Org. Chem.*, 1984, **49**, 1371 (*cmr, struct*)
Sardina, F.J. *et al*, *Chem. Lett.*, 1985, 697 (*struct*)
Coll, J.C. *et al*, *Aust. J. Chem.*, 1988, **41**, 1743 (*struct, cmr*)

Metachromin C M-80036



$C_{22}H_{30}O_4$ M 358.477
Constit. of *Hippospongia metachromia*. Yellow solid (hexane). Mp 90-91°. $[\alpha]_D^{26}$ −29.7° (c, 0.2 in $CHCl_3$).

Kabayashi, J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1173 (*isol, pmr, cmr*)

Methanetetrol M-80037

Tetra-O-benzyl: Tetrabenzyloxymethane. Tetrakis(phenylmethoxy)methane. Tetrabenzyl orthocarbonate. Benzyl orthocarbonate
$C_{29}H_{28}O_4$ M 440.538
Cryst. Mp 68-70°.

Latimer, D.R. *et al*, *Can. J. Chem.*, 1989, **67**, 143 (*synth, cryst struct, tetrabenzyl ester*)

Methanetricarboxaldehyde, 9CI M-80038

Triformylmethane
[18655-47-5]

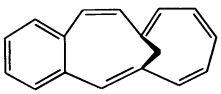
$$HC(CHO)_3 \rightleftharpoons HOCH{=}C(CHO)_2$$

$C_4H_4O_3$ M 100.074
Enol. from probable in solid state and Me_2CO but not $CHCl_3$ soln. Solid by subl. Mp 101-103°. pK_a 2.0.

Arnold, Z. *et al*, *Collect. Czech. Chem. Commun.*, 1960, **25**, 1318; 1961, **26**, 3051; 1965, **30**, 2125 (*synth, props*)
Arnold, Z. *et al*, *J. Org. Chem.*, 1988, **53**, 5352 (*synth*)
Keshavarz, K.M. *et al*, *Synthesis*, 1988, 641 (*synth, ir, uv, pmr, cmr, use, tautom, bibl*)

6,12-Methanobenzocyclododecene, 9CI M-80039

Updated Entry replacing B-60102
Benzo[c]-*1,7-methano*[*12*]*annulene*. *Benz*[b]*homoheptalene*
[84537-62-2]

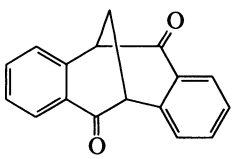


$C_{17}H_{14}$ M 218.298
Stable orange cryst. Mp 53-54°.

Scott, L.T. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 1372 (*synth, pmr, cmr, ir, uv*)
Günther, M.-G. *et al*, *Chem. Ber.*, 1986, **119**, 2942 (*pmr*)

5,11-Methanodibenzo[*a,e*]cyclooctene-6,12(5*H*,11*H*)dione, 9CI M-80040

2,3;6,7-Dibenzobicyclo[*3.3.1*]*nona-2,6-diene-4,8-dione*



(+)-*form*

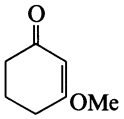
$C_{17}H_{12}O_2$ M 248.281
(+)-***form*** [59147-66-9]
$[\alpha]_D$ +139.5° (C, 0.021 in EtOH). 45% opt. pure.

(−)-***form***
Mp 195-197°. $[\alpha]_D^{22}$ −340° (c, 0.022 in EtOH).
(±)-***form*** [59147-65-8]
Needles (MeOH). Mp 147.7-147.8°.

Tatemitsu, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2473 (*synth, abs config*)
Naemura, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1989, **62**, 83.

3-Methoxy-2-cyclohexen-1-one M-80041

[16807-60-6]

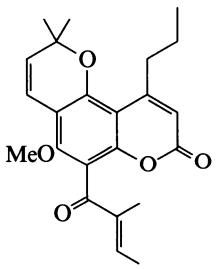


$C_7H_{10}O_2$ M 126.155
Liq. or cryst. (hexane). Mp 30-31°. Bp_{14} 114° ; $Bp_{0.7}$ 52-53° . n_D^{20} 1.5225.
(Z)-*oxime:* [29900-17-2].
Cryst. (H_2O). Mp 86.5-87°.
(E)-*4-Methylbenzenesulfonyloxime:* [32643-77-9].
Cryst. (ligroin). Mp 93-95°.
(Z)-*4-Methylbenzenesulfonyloxime:* [32643-76-8].
Powder (ligroin). Mp 78-82°.

Tamura, Y. *et al*, *Chem. Pharm. Bull.*, 1971, **19**, 523, 529 (*synth, ir, pmr*)
Cant, E. *et al*, *Bull. Soc. Chim. Belg.*, 1974, **83**, 93 (*ms*)
Lessard, J. *et al*, *Can. J. Chem.*, 1977, **55**, 1015 (*synth, pmr*)
Taskinen, E. *et al*, *Tetrahedron*, 1982, **38**, 613.
Pearson, A.J. *et al*, *J. Org. Chem.*, 1984, **49**, 3887 (*synth, ir, ms, pmr*)
Laurence, C. *et al*, *Spectrochim. Acta, Part A*, 1985, **41**, 883 (*ir, props*)
Imashiro, F. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 5213 (*cmr*)

5-Methoxy-2,2-dimethyl-6-(2-methyl-1-oxo-2-butenyl)-10-propyl-2*H*,8*H*-benzo-[1,2-*b*:3,4-*b*′]dipyran-8-one, 9CI M-80042

[39811-39-7]

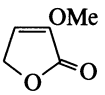


$C_{23}H_{26}O_5$ M 382.455
Isol. from *Calophyllum inophyllum*. Mp 121-123°.

Cavé, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **275**, 1105.

3-Methoxy-2(5*H*)-furanone M-80043

2-Methoxy-2-butenolide
[35214-62-1]

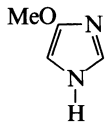


$C_5H_6O_3$ M 114.101

Isol. from *Narthecium ossifragum* flowering parts. Cryst. ($CHCl_3$). Mp 57°.

Stabursvik, A., *Acta Chem. Scand.*, 1954, **8**, 525 (*isol, struct, synth*)
Bonini, C.C. *et al*, *Org. Mass Spectrom.*, 1981, **16**, 68 (*ms*)

4(5)-Methoxyimidazole M-80044



$C_4H_6N_2O$ M 98.104
Cryst. Mp 115-116°.

Hosmane, R.S. *et al*, *J. Org. Chem.*, 1984, **49**, 1212 (*synth, pmr*)

Methoxy isocyanate M-80045

[117775-56-1]

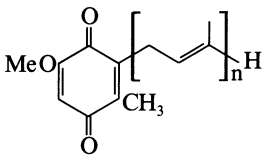
MeONCO

$C_2H_3NO_2$ M 73.051
Stable substance at −183°.

Teles, J.H., *Chem. Ber.*, 1989, **122**, 745 (*synth, ir*)

5-Methoxy-2-methyl-3-polyprenyl-1,4-benzoquinone M-80046

2-Polyprenyl-6-methoxy-3-methyl-1,4-benzoquinone



Isol. from *Rhodospirillum rubrum*. Intermed. in ubiquinone biosynth.

5-Methoxy-2-methyl-3-octaprenyl-1,4-benzoquinone [7200-29-5]
$C_{48}H_{72}O_3$ M 697.095
No phys. props. reported. n = 8.

5-Methoxy-2-methyl-3-nonaprenyl-1,4-benzoquinone [18735-22-3]
$C_{53}H_{80}O_3$ M 765.213
No phys. props. reported. n = 9.

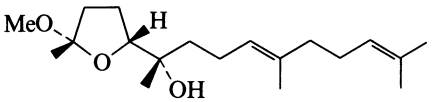
3- Decaprenyl-5-methoxy-2-methyl-1,4-benzoquinone [7200-27-3]
$C_{58}H_{88}O_3$ M 833.331
No phys. props. reported. n = 10. λ_{max} 266, 274sh nm.

Friis, P. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 4754 (*isol, ms, struct*)

2-(5-Methoxy-5-methyltetrahydro-2-furanyl)-6,10-dimethyl-5,9-undecadien-2-ol M-80047

α-(4,8-Dimethyl-3,7-nonadienyl)tetrahydro-5-methoxy-α,5-dimethyl-2-furanmethanol, 9CI

[115028-54-1]



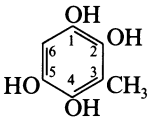
$C_{19}H_{34}O_3$ M 310.476
Constit. of *Cystophora moniliformis*. Oil. $[\alpha]_D$ +11° (c, 1.3 in $CHCl_3$).

van Altena, I.A., *Aust. J. Chem.*, 1988, **41**, 49.

3-Methyl-1,2,4,5-benzenetetrol M-80048

2,3,5,6-Tetrahydroxytoluene

[700-19-6]



$C_7H_8O_4$ M 156.138

1-Me ether: 5-Methoxy-3-methyl-1,2,4-benzenetriol. 2,3,6-Trihydroxy-5-methoxytoluene
$C_8H_{10}O_4$ M 170.165
Prisms by subl. Mp 102-103°. Darkens in air.

1-Me ether, Tri-Ac:
$C_{14}H_{16}O_7$ M 296.276
Hexagonal plates (MeOH). Mp 155°.

Anslow, W.K. *et al*, *J. Chem. Soc.*, 1939, 1446.

4-Methyl-1,2,3,5-benzenetetrol M-80049

2,3,4,6-Tetrahydroxytoluene

$C_7H_8O_4$ M 156.138

1-Me ether: 6-Methoxy-3-methyl-1,2,4-benzenetriol. 2,3,6-Trihydroxy-4-methoxytoluene
$C_8H_{10}O_4$ M 170.165
Cryst. by subl. Mp 150°.

3-Me ether: 6-Methoxy-5-methyl-1,2,4-benzenetriol. 3,4,6-Trihydroxy-2-methoxytoluene
$C_8H_{10}O_4$ M 170.165
Cryst. by subl. Mp 146-147°.

3-Me ether, tri-Ac:
$C_{14}H_{16}O_7$ M 296.276
Plates (MeOH). Mp 98-99°.

Anslow, W.K. *et al*, *J. Chem. Soc.*, 1938, 469.

5-Methyl-1,2,3,4-benzenetetrol, 9CI M-80050

Updated Entry replacing M-00966

2,3,4,5-Tetrahydroxytoluene. 5-Methylapionol

[700-20-9]

$C_7H_8O_4$ M 156.138
Isol. from submerged cultures of *Aspergillus fumigatus*. Cryst. (toluene). Mp 170-171° (140°). Darkens in air.

Tetra-Ac:
$C_{15}H_{16}O_8$ M 324.287
Cryst. (MeOH). Mp 132-133°.

2-Me ether: 3-Methoxy-6-methyl-1,2,4-benzenetriol. ***Dihydrofumigatin***
$C_8H_{10}O_4$ M 170.165
Metab. of *A. fumigatus*. Needles by subl.

2-Me, 1,3,4-tri-Ac: Mp 91-92°.

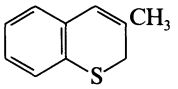
Tetra-Me ether: [35896-58-3]. *1,2,3,4-Tetramethoxy-5-methylbenzene*
$C_{11}H_{16}O_4$ M 212.245
Mp 51-52°.

Thiele, J. *et al*, *Justus Liebigs Ann. Chem.*, 1900, **311**, 341 (*synth*)
Erdtman, H.G.H., *Proc. R. Soc. London, A*, 1934, **143**, 177; *CA*, **38**, 1337 (*synth*)
Anslow, W.K. *et al*, *Biochem. J.*, 1938, **32**, 687 (*Dihydrofumigatin*)
Packter, N.M., *Biochem. J.*, 1966, **98**, 353 (*isol, synth, deriv*)
Syper, L. *et al*, *Tetrahedron*, 1980, **36**, 123 (*deriv*)
Keinan, E. *et al*, *J. Org. Chem.*, 1987, **52**, 3872 (*synth, deriv*)

3-Methyl-2*H*-1-benzothiopyran, 9CI M-80051

*3-Methyl-2*H*-1-benzothiin. 3-Methyl-2*H*-thiochromene*

[6157-11-5]



$C_{10}H_{10}S$ M 162.255

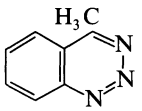
Oil. Bp_5 110-115°.

Tilak, B.D. *et al*, *Tetrahedron*, 1966, **22**, 7 (*synth*)
Arnoldi, A. *et al*, *Synthesis*, 1988, 155 (*synth, pmr*)

4-Methyl-1,2,3-benzotriazine, 9CI M-80052

Updated Entry replacing M-30058

[33334-15-5]



$C_8H_7N_3$ M 145.163

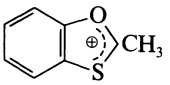
Prisms (EtOH). Mp 120-121°. λ_{max} 207 (log ϵ 3.58), 2.27(4.0) and 275 nm (2.83) (EtOH).

2-Oxide:
$C_8H_7N_3O$ M 161.163
Cryst. (CH_2Cl_2/pet. ether or by subl.). Mp 176-178°.

3-Oxide: [41608-06-4].
$C_8H_7N_3O$ M 161.163
Orange-yellow plates (EtOH) or cryst. (C_6H_6). Mp 185-188° dec. (175-177°). Dec. in daylight.

Meisenheimer, J. *et al*, *Ber.*, 1927, **60**, 1736 (*oxide*)
Adger, B.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 31 (*synth, ir, uv, pmr*)
Boulton, A.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1509 (*oxides*)

2-Methyl-1,3-benzoxathiazolium(1+) M-80053



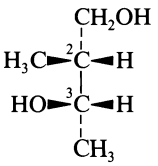
$C_8H_7OS^{\oplus}$ M 151.209 (ion)

Tetrafluoroborate: [112816-51-0].
$C_8H_7BF_4OS$ M 238.013
Cryst. Mp 87-88° dec. Moisture sensitive.

Barbero, M. *et al*, *J. Org. Chem.*, 1988, **53**, 2245 (*synth, pmr, cmr*)

2-Methyl-1,3-butanediol M-80054

[684-84-4]



(2*R*,3*S*)-*form*

$C_5H_{12}O_2$ M 104.149

(2RS,3SR)-form [87678-97-5]
(+)-erythro-*form*
$[\alpha]_D^{20}$ +3.5° (c, 1.7 in EtOH).

(2S,3R)-form [90026-43-0]
(−)-erythro-*form*
Bp_{15} 110°. $[\alpha]_D$ −6.3°.

(2RS,3RS)(?)-form [16897-85-1]
(±)-threo-*form*
n_D^{20} 1.4465. May be the (±)-erythro-form. The 2 racemates have been distinguished and characterised spectroscopically but no phys. props. were given.

Bis-p-nitrobenzoyl: Mp 128°.

(2RS,3SR)-(?)-form [16897-83-9]
(±)-erythro-*form*
n_D^{20} 1.4500.

*Bis-*p*-nitrobenzoyl:* Mp 113°.

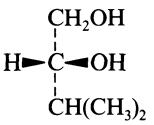
[90026-54-3, 98048-91-0]

Fremaux, B. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 4243 (*synth*)
Dolby, L.J. *et al*, *J. Org. Chem.*, 1968, **33**, 3060 (*synth, pmr*)
Nájera, C. *et al*, *Helv. Chim. Acta*, 1984, **67**, 289 (*synth, pmr*)
White, J.D. *et al*, *J. Org. Chem.*, 1988, **53**, 5909 (*synth, ir, pmr, cmr, ms*)

3-Methyl-1,2-butanediol M-80055

Isopropylethyleneglycol

[50468-22-9]



(*R*)-*form*

$C_5H_{12}O_2$ M 104.149

(R)-form [31612-62-1]
Liq. Bp_7 88°. $[\alpha]_D^{20}$ −6.4° (c, 1.46 in cyclohexane), $[\alpha]_D$ −10.95° (c, 1 in $CHCl_3$) (100% opt. purity).

(S)-form [24347-56-6]
Liq. Bp_3 75.5°. $[\alpha]_D^{25}$ +6.32° (c, 2 in cyclohexane).

[63163-20-2]

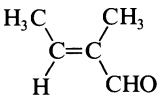
Bartlett, P.D. *et al*, *J. Biol. Chem.*, 1937, **118**, 503 (*synth*)
Fuganti, C. *et al*, *Gazz. Chim. Ital.*, 1969, **99**, 316 (*abs config*)
Guetté, J.-P. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 4217 (*synth, abs config*)
Tsuji, K. *et al*, *Makromol. Chem. Suppl.*, 1975, **1**, 55 (*synth*)
White, J.D. *et al*, *J. Org. Chem.*, 1988, **53**, 5909 (*synth, ir, pmr, cmr, ms*)

2-Methyl-2-butenal, 9CI M-80056

Updated Entry replacing M-01205

2,3-Dimethylacrolein. 2-Methylcrotonaldehyde

[1115-11-3]



(*E*)-*form*

C_5H_8O M 84.118

(E)-form [497-03-0]
Tiglic aldehyde. Tiglaldehyde
Isol. from *Allium schoenoprasum* (chives). Spar. sol. H_2O. Bp 116.5-117.5°, Bp_{119} 63.2-65.0°.

2,4-Dinitrophenylhydrazone: Red cryst. (EtOAc/Me_2CO). Mp 215.5-217.5° (222°).

Oxime:
C_5H_9NO M 99.132
Cryst. (Et_2O). Mp 43°.

Semicarbazone: Needles (EtOH). Mp 219° (234°).

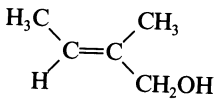
(Z)-form [6038-09-1]
Angelic aldehyde
Liq. Isom. to *E*-form after 2 weeks at r.t.

[6038-09-1]

Wahlroos, O. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1327 (*isol*)
Satsumabayashi, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 1586 (*synth, ir*)
Botteghi, C. *et al*, *Tetrahedron Lett.*, 1974, 4285 (*synth*)
Vögeli, U. *et al*, *Org. Magn. Reson.*, 1975, **7**, 617 (*synth, pmr, cmr, isom*)
Loewenthal, H.J.E., *Synth. Commun.*, 1975, **5**, 201 (*synth*)
Eletti-Bianchi, G. *et al*, *J. Org. Chem.*, 1976, **41**, 1648 (*synth*)
Kieczykowski, G.R. *et al*, *Tetrahedron Lett.*, 1976, 597 (*synth*)

2-Methyl-2-buten-1-ol, 9CI M-80057

[4675-87-0]



(*E*)-*form*

$C_5H_{10}O$ M 86.133

Widespread nat. occurrence, e.g. in *Ochromonas danica*, in *Anthemis nobilis* (as acetate), in fruit juices and animal sources (unspecified stereochem.). Bp_{30} 68-70°.

(***E*)-*form*** [497-02-9]

Tiglic alcohol. Tiglyl alcohol

Formed in *Anthemis nobilis* (together with esters). Bp 122-127° (135°) , Bp_{33} 66°.

(***Z*)-*form*** [19319-26-7]

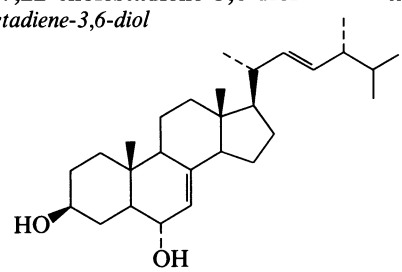
Angelic alcohol. Angelyl alcohol

Bp 136-137°, Bp_{25} 61-63°. n_D^{20} 1.4410.

Katzenellenbogen, J.A. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 4925 (*synth, ir, pmr*)
Jarolim, V. *et al*, *Collect. Czech. Chem. Commun.*, 1977, **42**, 3490 (*synth*)
Zaidlewicz, M. *et al*, *Synthesis*, 1979, 62 (*synth, pmr*)
Depezay, J.-C. *et al*, *Bull. Soc. Chim. Fr.*, 1981, 306 (*synth, ms, pmr*)
Smith, P.A.S. *et al*, *J. Org. Chem.*, 1981, **46**, 3970 (*synth, ir, pmr*)
Bury, A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1982, 645 (*synth, pmr*)
Masami, Y. *et al*, *Tetrahedron*, 1984, **40**, 3481 (*synth, ir, pmr*)
Ono, N. *et al*, *Tetrahedron Lett.*, 1984, **25**, 5319 (*synth*)
Trost, B.M. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 1293 (*synth, pmr*)
Kurth, M.J. *et al*, *J. Org. Chem.*, 1985, **50**, 5769 (*synth*)
Ashcroft, M.R. *et al*, *J. Organomet. Chem.*, 1985, **289**, 403 (*synth*)
Simon, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 785 (*synth*)
Bicchi, C. *et al*, *J. Chromatogr.*, 1987, **411**, 237 (*glc, ms*)

24-Methyl-7,22-cholestadiene-3,6-diol M-80058

7,22-Ergostadiene-3,6-diol



$C_{28}H_{46}O_2$ M 414.670

(***3β,5α,6α,22E,24R*)-*form***

Constit. of *Spongionella gracilis*. Cryst. (MeOH/pet. ether). Mp 206-208°.

(***3β,5α,6α,22E,24S*)-*form***

Constit. of *S. gracilis*. Cryst. (MeOH/pet. ether). Mp 196-198°.

Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol, pmr*)

24-Methyl-7,22-cholestadien-3-ol M-80059

Updated Entry replacing M-01279

7,22-Ergostadien-3-ol

$C_{28}H_{46}O$ M 398.671

(***3β,5α,22E,24R*)-*form*** [2465-11-4]

Stellasterol

Constit. of wood-rotting fungi. Cryst. (CH_2Cl_2/MeOH). Mp 159.5-161°. $[\alpha]_D$ −17.8° ($CHCl_3$).

(***3β,5α,22E,24S*)-*form*** [50364-22-2] ***5,6-Dihydroergosterol***

Constit. of *Tylopitus neofelleus* and *Polyporus umbellatus*. Constit. of yeast and grapefruit oil. Cryst. (MeOH). Mp 173.5-174°. $[\alpha]_D$ −23.4°.

3-Ketone: 24-Methyl-7,22-cholestadien-3-one. 7,22-Ergostadien-3-one

$C_{28}H_{44}O$ M 396.655

Constit. of *Fomes formentarius*. Cryst. (Me_2CO). Mp 184-186°. $[\alpha]_D$ +6° ($CHCl_3$).

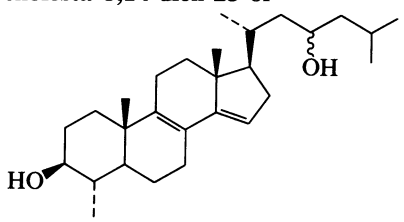
3-O-β-D-Glucopyranoside:

$C_{34}H_{56}O_6$ M 560.813

Constit. of *T. neofelleus*. Needles (MeOH). Mp 272-274°. $[\alpha]_D^{22}$ +31.1° (c, 0.9 in Py).

Callow, R.K., *Biochem. J.*, 1931, **25**, 87 (*isol*)
Arthur, H.R. *et al*, *J. Chem. Soc.*, 1958, 2603 (*isol*)
Kobayashi, M. *et al*, *Tetrahedron*, 1973, **29**, 1193 (*isol*)
Bélanger, P. *et al*, *Can. J. Chem.*, 1973, **51**, 3294 (*biosynth*)
Rubinstein, I. *et al*, *Phytochemistry*, 1976, **15**, 195 (*pmr*)
Lu, W. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 5083 (*isol*)
Takaishi, Y. *et al*, *Phytochemistry*, 1989, **28**, 945 (*isol, deriv*)

4-Methylcholesta-8,14-dien-23-ol M-80060



$C_{28}H_{46}O_2$ M 414.670

(***4α,23ξ*)-*form***

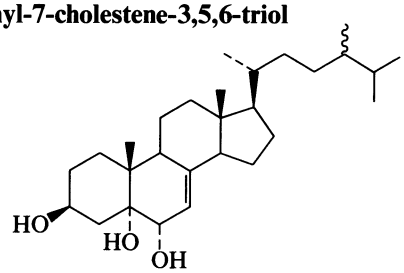
3-O-[β-D-Galactopyranosyl(1→2)-β-D-galactopyranoside]: [119760-82-6]. ***Eryloside A***

$C_{40}H_{66}O_{12}$ M 738.954

Constit. of *Erylus lendenfeldi*. Shows antitumour and antifungal props. Amorph. powder. Mp 214-219°. $[\alpha]_D$ +11° (c, 1.5 in $CHCl_3$).

Carmely, S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 167 (*isol, pmr, cmr*)

24-Methyl-7-cholestene-3,5,6-triol M-80061



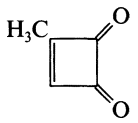
$C_{28}H_{48}O_3$ M 432.685

(***3β,5α,6α,24ξ*)-*form***

Constit. of *Hippospongia communis*, *Spongia officinalis* and *Ircinia variabilis*.

Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol, pmr*)

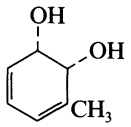
3-Methyl-3-cyclobutene-1,2-dione M-80062



$C_5H_4O_2$ M 96.085
Golden liq. $Bp_{3.6}$ 68-70°.

Liebeskind, L.S. *et al*, *J. Org. Chem.*, 1988, **53**, 2482 (*synth, ir, pmr*)

3-Methyl-3,5-cyclohexadiene-1,2-diol, 9CI M-80063



(1*S*,2*R*)-*form*

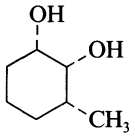
$C_7H_{10}O_2$ M 126.155

(1S,2R)-form [41977-20-2]
(+)-cis-*form*
Product of oxidation of toluene by a mutant of *Pseudomonas putida*, a soil bacterium. Prostaglandin synthon. Cryst. (pet. ether). Mp 59°. $[\alpha]_D^{25}$ +26.4° (c, 0.38 in MeOH).

Gibson, D.T. *et al*, *Biochemistry*, 1970, **9**, 1626 (*isol, uv, ir, pmr*)
Ziffer, H. *et al*, *Tetrahedron*, 1977, **33**, 2491 (*abs config*)
Hudlicky, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4735 (*synth, ir, pmr*)

3-Methyl-1,2-cyclohexanediol, 9CI M-80064

[23477-91-0]



(1*S*,2*R*,3*R*)-*form*

$C_7H_{14}O_2$ M 130.186

(1S,2R,3R)-form [41977-21-3]
(−)-cis,cis-form
Oil. $[\alpha]_D^{20}$ −37° (c, 0.97 in MeOH).

1-Benzoyl: Cryst. Mp 84-85°. $[\alpha]_D^{20}$ −25° (c, 1.05 in $CHCl_3$).

1,2-Dibenzoyl: Oil.

(1RS,2RS,3SR)-form [15806-70-9]
(±)-trans,trans-form
Mp 39-40°.

(1RS,2RS,3RS)-form [19700-12-0]
(±)-trans,cis-form
Cryst. (2,2-dimethylpentane). Mp 94-95°.

(1RS,2SR,3RS)-form [19700-14-2]
(±)-cis,trans-form
Cryst. (hexane/EtOAc). Mp 81-82°.

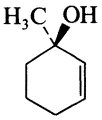
(1RS,2SR,3SR)-form [52730-58-2]
(±)-cis,cis-form
Cryst. (hexane/EtOAc). Mp 64-65°.

[41977-22-4]

Klein, J. *et al*, *Tetrahedron*, 1968, **24**, 5701 (*synth, pmr, ir*)
Ziffer, H. *et al*, *J. Org. Chem.*, 1974, **39**, 3698 (*synth, cmr*)
Ziffer, H. *et al*, *Tetrahedron*, 1977, **33**, 2491 (*synth, pmr, abs config*)
Hudlicky, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4735 (*synth, ir, pmr*)

1-Methyl-2-cyclohexen-1-ol, 9CI M-80065

Updated Entry replacing M-01411
[23758-27-2]



(*R*)-*form*

$C_7H_{12}O$ M 112.171
Component of the aggregation pheromone of the douglas fir beetle *Dendroctonus psuedotsugae*.

(R)-form [88494-89-7]
Bp_{16} 60°. $[\alpha]_D^{23}$ +75.8° (c, 1.0 in Et_2O). n_D^{20} 1.4730.

(S)-form [112837-29-3]
Bp_{16} 60°. $[\alpha]_D^{23}$ −76.5° (c, 8.50 in Et_2O). n^{20} 1.4705.

(±)-form
Bp_{23} 110°, Bp_{15} 60-61°.

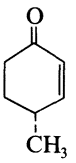
Ac:
$C_9H_{14}O_2$ M 154.208
$Bp_{0.4}$ 85°.

4-Nitrobenzoyl: [38313-13-2].
Cryst. (hexane). Mp 101-102°.

Mandrou, A.-M. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 1546 (*synth*)
Magnusson, G. *et al*, *J. Org. Chem.*, 1973, **38**, 1380 (*synth, cmr*)
Beckwith, A.L.J. *et al*, *Aust. J. Chem.*, 1976, **29**, 1277 (*synth*)
Mori, K. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 903 (*synth, bibl*)

4-Methyl-2-cyclohexen-1-one, 9CI M-80066

Updated Entry replacing M-20108
[5515-76-4]



(*R*)-*form*

$C_7H_{10}O$ M 110.155

(R)-form [75337-05-2]
Oil. Bp 198°. $[\alpha]_D^{22}$ +105° (c, 9.2 in $CHCl_3$).

(S)-form
Chiral synthon. $[\alpha]_D^{22}$ −199° (c, 0.37 in EtOH).

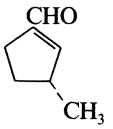
(±)-form
Liq. Bp 175-176°, Bp_{13} 81-85°. Steam-volatile.

2,4-Dinitrophenylhydrazone: [3280-41-9].
Dark-red cryst. Mp 173-174°.

Kötz, A. *et al*, *Justus Liebigs Ann. Chem.*, 1913, **400**, 86 (*synth*)
Birch, A.J., *J. Chem. Soc.*, 1946, 593 (*synth*)
Torri, J. *et al*, *Tetrahedron Lett.*, 1973, 3251 (*uv*)
Barieux, J.J. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 1020 (*cmr*)
Torri, J. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 1633 (*cmr*)
Silvestri, M.G., *J. Org. Chem.*, 1983, **48**, 2419 (*synth, pmr*)
Hiroi, K. *et al*, *Synthesis*, 1985, 635 (*synth*)
Hua, D.H. *et al*, *J. Org. Chem.*, 1988, **53**, 1095 (*synth, ir, pmr, cmr*)

3-Methyl-1-cyclopentenecarboxaldehyde M-80067

1-Formyl-3-methylcyclopentene
[90049-64-2]



(*R*)-*form*

$C_7H_{10}O$ M 110.155

Terpene synthon.

(R)-form [114818-64-3]

Bp_2 30° (Kugelrohr) . $[\alpha]_D^{25}$ +193.3° (c, 1.058 in $CHCl_3$).

(S)-form [114818-65-4]

$[\alpha]_D^{25}$ −214.9° (c, 0.1 in $CHCl_3$).

(±)-form

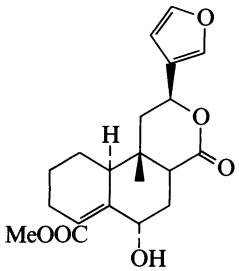
Liq. Bp_{16} 56-57°.

2,4-Dinitrophenylhydrazone: Mp 175-183°.

Semicarbazone: Mp 178-180°.

Garanti, L. *et al*, *Ann. Chim. (Rome)*, 1963, **53**, 1619 (*synth*)
Hudlicky, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4735 (*synth, ir, pmr*)

Methyl 12,17;15,16-diepoxy-6-hydroxy-19-nor-17-oxo-4,13(16),14-clerodatrien-18-oate M-80068



$C_{20}H_{24}O_6$ M 360.406

Not named in the paper.

O-β-D-Glucopyranoside:

$C_{26}H_{34}O_{11}$ M 522.548

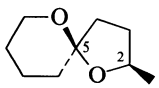
Constit. of *Tinospora cordifolia*. Cryst. Mp 199-201°. $[\alpha]_D^{70}$ +23.8° (c, 3.14 in MeOH).

Bhatt, R.K. *et al*, *Phytochemistry*, 1989, **28**, 2419.

7-Methyl-1,6-dioxaspiro[4.5]decane M-80069

Updated Entry replacing M-20115

[68108-91-8]



(2R,5R)-form

$C_9H_{16}O_2$ M 156.224

Main component of the odour of the common wasp, *Paravespula vulgaris* which appears to act as aggression inhibitor. Ident. by glc/ms.

(2R,5R)-form

Bp_{20} 100-110° (bath) . $[\alpha]_D^{20}$ −83.4° (c, 0.718 in pentane).

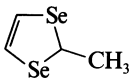
(2S,5R)-form

Bp_{20} 100-110° (bath) . $[\alpha]_D^{20}$ −79.1° (c, 0.392 in pentane). The enantiomeric (2*S*,5*S*) and (2*R*,5*S*)-forms also prepd.

Erdmann, H., *Justus Liebigs Ann. Chem.*, 1885, **228**, 176 (*synth*)
Francke, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1978, **17**, 862 (*isol, synth*)
Jacobson, R. *et al*, *J. Org. Chem.*, 1982, **47**, 3140 (*synth*)
Ley, S.V. *et al*, *Tetrahedron Lett.*, 1984, **25**, 113 (*synth*)
Iwata, C. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4785 (*synth, pmr*)

2-Methyl-1,3-diselenole M-80070

[115118-34-8]



$C_4H_6Se_2$ M 212.011

Low melting solid. Mp 30°.

Lakshmikantham, M.V. *et al*, *J. Org. Chem.*, 1988, **53**, 3529 (*synth, pmr, ms*)

2-Methyldotriacontane, 9CI M-80071

[1720-11-2]

$H_3C(CH_2)_{29}CH(CH_3)_2$

$C_{33}H_{68}$ M 464.900

Isol. from leaf wax of *Aeonium lindleyi* and *Nicotiana* sp.. Present in surface lipids of pupal tobacco budworms (*Heliothis virescens*), in sex pheromones of insect spp. and in camomile wax.

[69067-11-4]

Eglington, D. *et al*, *Phytochemistry*, 1966, **5**, 1349 (*isol, ir, ms*)
Guelz, P.G. *et al*, *Phytochemistry*, 1968, **7**, 1009 (*isol, ms*)
Gamou, K. *et al*, *Agric. Biol. Chem.*, 1980, **44**, 2119 (*isol, glc*)
Heeman, V. *et al*, *Phytochemistry*, 1983, **22**, 133 (*isol, ms*)

3-Methyldotriacontane, 9CI M-80072

[20129-49-1]

$H_3C(CH_2)_{28}CH(CH_3)CH_2CH_3$

$C_{33}H_{48}$ M 444.742

Present in leaves and chloroplasts of *Antirrhinum majus*, in *Nicotiana* sp. and in cuticular membranes of insect spp.

Guelz, P.G. *et al*, *Phytochemistry*, 1968, **7**, 1009 (*isol, glc, ms*)
Heeman, V. *et al*, *Phytochemistry*, 1983, **22**, 133 (*isol, ms*)

6-Methyldotriacontene, 9CI M-80073

[92122-78-6]

$H_3C(CH_2)_{25}CH(CH_3)CH_2CH_2CH_2CH_2CH_3$

$C_{33}H_{68}$ M 464.900

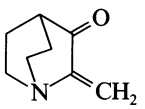
Isol. from leaves and stems of *Duboisia myoporoides*.

Shukla, Y.N. *et al*, *Phytochemistry*, 1984, **23**, 799 (*isol, struct*)

2-Methylene-1-azabicyclo[2.2.2]octan-3-one M-80074

2-Methylene-3-quinuclidinone

[5291-26-9]



$C_8H_{11}NO$ M 137.181

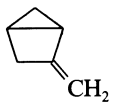
Slightly yellow oil. Bp_7 91-92°, $Bp_{0.5}$ 80°.

B,HCl: Cryst. (Et_2O). Mp 243-244° dec.

Hansen, A.R. *et al*, *J. Heterocycl. Chem.*, 1966, **3**, 109 (*synth, ir*)
Morgan, T.K. *et al*, *J. Med. Chem.*, 1987, **30**, 2259 (*synth, pmr*)

2-Methylenebicyclo[2.1.0]pentane, 9CI M-80075

[116377-11-8]



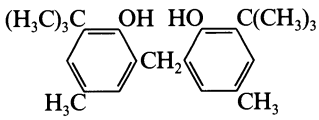
C_6H_8 M 80.129

Andrews, G.D. *et al*, *J. Org. Chem.*, 1988, **53**, 4624 (*synth, pmr, props*)

2,2′-Methylenebis[6-*tert*-butyl-4-methylphenol] M-80076

2,2′-Methylenebis[6-(1,1-dimethylethyl)-4-methylphenol], 9CI.
*2,2′-Methylenebis[6-*tert*-butyl-p-cresol], 8CI*

[119-47-1]



$C_{23}H_{32}O_2$ M 340.505

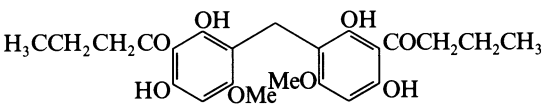
Polymer antioxidant. Needles (pet. ether). Mp 131°.

Hultzsch, K., *J. Prakt. Chem.*, 1941, **159**, 155, 178 (*synth*)
Coggeshall, N.D. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 3283; 1950, **72**, 2836 (*ir, uv*)
Wextler, A.S., *Anal. Chem.*, 1963, **35**, 1936 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., 1978-1984, *Wiley, NY*, 3rd Ed., Wiley, N.Y., 1968-1984, **3**, 130 (*use*)
Lesko, J. *et al*, *Collect. Czech. Chem. Commun.*, 1969, **34**, 2836 (*ms*)

Methylenebisdesaspidinol BB M-80077

1,1′-[Methylenebis(2,6-dihydroxy-4-methoxy-3,1-phenylene)]bis-1-butanone, 9CI

[32190-32-2]



$C_{23}H_{28}O_8$ M 432.469

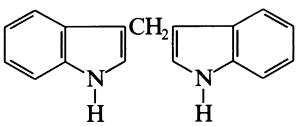
The BB suffix refers to the two butanoyl side-chains. In theory other methylenebisaspidinols could occur naturally. Isol. from *Dryopteris* spp. ferns. Mp 176-179°.

Penttilä, A. *et al*, *Acta Chem. Scand.*, 1963, **17**, 1886.
Widén, C.-J. *et al*, *Helv. Chim. Acta*, 1971, **54**, 2824.

3,3′-Methylenebisindole, 9CI M-80078

3,3′-Methylenediindole. Di-3-indolylmethane

[1968-05-4]



$C_{17}H_{14}N_2$ M 246.311

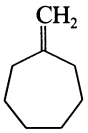
Needles (EtOH aq.). Mp 165-166°.

1,1′-Di-Me: [31896-75-0].
$C_{19}H_{18}N_2$ M 274.365
Plates (EtOH). Mp 110-112°.

Thesing, J., *Chem. Ber.*, 1954, **87**, 692 (*synth*)
Jackson, A.H. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 2543 (*synth, pmr*)

Methylenecycloheptane M-80079

[2505-03-5]



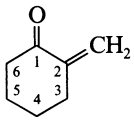
C_8H_{14} M 110.199

d_{20} 0.83. Bp 133° (138-140°) .

Wallach, O., *Justus Liebigs Ann. Chem.*, 1906, **345**, 139 (*synth*)
Šorm, F. *et al*, *Chem. Listy*, 1953, **47**, 708 (*synth*)
Donaldson, W.A., *Tetrahedron*, 1987, **43**, 2901 (*synth*)

2-Methylenecyclohexanone, 9CI, 8CI M-80080

[3045-98-5]



$C_7H_{10}O$ M 110.155

Liq. Dimerises rapidly at r.t.

Semicarbazone: Needles (EtOH). Mp 210° dec.

Di-Et ketal: [23153-78-8]. *1,1-Diethoxy-2-methylenecylohexane*
$C_{11}H_{20}O_2$ M 184.278
Bp_{12} 77-78°.

Mannich, C. *et al*, *Chem. Ber.*, 1941, **74**, 555 (*synth*)
Erskine, R.L. *et al*, *J. Chem. Soc.*, 1960, 3425 (*ir*)
Mühlstädt, M. *et al*, *J. Prakt. Chem.*, 1965, **29**, 158; 1970, **312**, 292 (*synth, pmr*)
Kirmse, W. *et al*, *Chem. Ber.*, 1969, **102**, 2440 (*ketal, synth, pmr*)
Bravo, P. *et al*, *Gazz. Chim. Ital.*, 1969, **99**, 549 (*oxime, synth, ir, pmr, ms*)
Ksander, G.M. *et al*, *J. Org. Chem.*, 1977, **42**, 1180 (*synth*)
Fleming, I. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1493 (*synth*)

3-Methylenecyclohexanone, 9CI, 8CI M-80081

$C_7H_{10}O$ M 110.155

Di-Me ketal: [104598-80-3]. *1,1-Dimethoxy-3-methylenecyclohexane*
$C_9H_{16}O_2$ M 156.224
Liq.

Ethylene ketal: [104598-81-4]. *7-Methylene-1,4-dioxaspiro[4.5]decane*
$C_9H_{14}O_2$ M 154.208
Liq.

Lambert, J.B. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 7575 (*synth, pmr, uv*)

4-Methylenecyclohexanone, 9CI, 8CI M-80082

[29648-66-6]

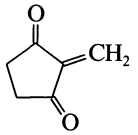
$C_7H_{10}O$ M 110.155

Bp_{15} 70-80°.

2,4-Dinitrophenylhydrazone: Cryst. Mp 154-155°.

Ooba, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 1782 (*ir, ms, pmr*)
Sonoda, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 1777 (*synth*)
Coughlin, D.J. *et al*, *J. Org. Chem.*, 1979, **44**, 3784 (*synth, pmr*)

2-Methylene-1,3-cyclopentanedione M-80083

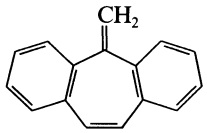


$C_6H_6O_2$ M 110.112
Intermediate trapped as Diels-Alder adduct.

Eaton, P.E. *et al*, *Can. J. Chem.*, 1984, **62**, 2612 (*synth*)
Bunnelle, W.H. *et al*, *Tetrahedron*, 1987, **43**, 2005 (*synth*)

5-Methylene-5*H*-dibenzo[*a,d*]cycloheptene, 9CI M-80084

1-Methylene-2,3:6,7-dibenz-4-suberene
[2975-79-3]

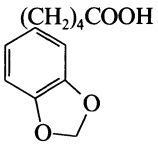


$C_{16}H_{12}$ M 204.271
Cryst. (EtOH). Mp 119-121°.

Triebs, W. *et al*, *Ber.*, 1951, **84**, 671 (*synth*)
Granoth, I. *et al*, *J. Org. Chem.*, 1976, **41**, 3682 (*synth*)
Lamanec, T.R. *et al*, *J. Org. Chem.*, 1988, **53**, 1768 (*synth, pmr*)

5-(3,4-Methylenedioxyphenyl)pentanoic acid M-80085

1,3-Benzodioxole-5-pentanoic acid, 9CI. Piperhydronic acid. Tetrahydropiperinic acid
[41917-45-7]



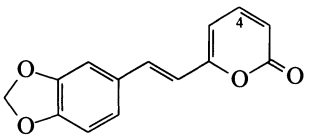
$C_{12}H_{14}O_4$ M 222.240
Isol. from fruits of *Piper longum*. Tablets or platelets (EtOH). Mp 100-101° (90-91°).

Et ester: Bp_1 155°.

Gokhale, V.G. *et al*, *CA*, 1949, **43**, 1085 (*isol*)
Viswanathan, N. *et al*, *Helv. Chim. Acta*, 1975, **58**, 2026 (*synth*)

6-(3,4-Methylenedioxystyryl)-α-pyrone M-80086

6-[2-(1,3-Benzodioxol-5-yl)ethenyl]-2H-pyran-2-one, 9CI
[1219-50-7]



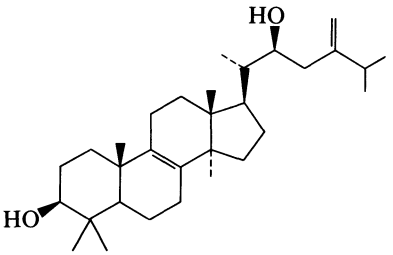
$C_{14}H_{10}O_4$ M 242.231
Isol. from wood of *Aniba parviflora*. Yellow cryst. (C_6H_6). Mp 173-174°.

4-Methoxy: 4-Methoxy-6-(3,4-methylenedioxystyryl)-α-pyrone. 5,6-Dehydromethysticin
$C_{15}H_{12}O_5$ M 272.257
Isol. from wood of *A. heringeri*. Light yellow-green cryst. Mp 233-234°.

[31983-44-5]

Mors, W.B. *et al*, *An. Assoc. Quim. Bras.*, 1962, **21**, 7 (*deriv*)
Gottlieb, O.R. *et al*, *Ann. Acad. Bras. Cienc.*, 1964, **36**, 29 (*isol, ir, struct*)
Mahajan, J.R. *et al*, *J. Org. Chem.*, 1971, **36**, 1832 (*synth*)

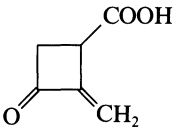
24-Methylene-8-lanostene-3,22-diol M-80087



$C_{31}H_{52}O_2$ M 456.751
(3β,22S)-form [119513-64-3]
Metab. of *Pisolithus tinctorius*. Cryst. (MeOH). Mp 161-165°. $[\alpha]_D$ +29° (c, 0.16 in $CHCl_3$).

Lobo, A.M. *et al*, *Phytochemistry*, 1988, **27**, 3569.

2-Methylene-3-oxocyclobutanecarboxylic acid M-80088



$C_6H_6O_3$ M 126.112
(±)-form
Me ester: [112139-41-0].
$C_7H_8O_3$ M 140.138
Oil.

Vidal, J. *et al*, *J. Org. Chem.*, 1988, **53**, 611 (*synth, pmr, cmr, ir, uv, ms*)

2-Methylenepentanedinitrile, 9CI M-80089

2-Methyleneglutaronitrile, 8CI. 2,4-Dicyano-1-butene
[1572-52-7]

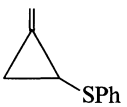
$H_2C{=}C(CN)CH_2CH_2CN$

$C_6H_6N_2$ M 106.127
Dimer of acrylonitrile. Liq. d^{20} 0.976. Mp −9.6°. Bp 103°. n_D^{20}1.4559.

Aldrich Library of FT-IR Spectra, 1st Ed., **1**, 844D (*ir*)
Aldrich Library of NMR Spectra, 2nd Ed., **2**, 702D (*pmr*)
Sadtler Standard Infrared Spectra, No. 34514 (*ir*)
Sadtler Standard NMR Spectra, No. 5428 (*pmr*)
Baizer, M.M. *et al*, *J. Org. Chem.*, 1965, **30**, 1357 (*synth, props*)
Price, P. *et al*, *Anal. Chem.*, 1976, **48**, 494 (*ms*)
Basaraiah, D. *et al*, *Tetrahedron Lett.*, 1987, **28**, 4591 (*synth*)

1-Methylene-2-(phenylthio)cyclopropane M-80090

[(Methylenecyclopropyl)thio]benzene, 9CI. 1-Methylidene-2-(phenylthio)cyclopropane
[78656-80-1]



$C_{10}H_{10}S$ M 162.255
(±)-form
Light-yellow oil. $Bp_{0.01}$ 65°.

S-*Oxide:* [94923-10-1]. *1-Methylene-2-(phenylsulfinyl)cyclopropane. 1-Methylidene-2-(phenylsulfinyl)cyclopropane. [(Methylenecyclopropyl)sulfinyl]benzene, 9CI*
$C_{10}H_{10}OS$ M 178.254
Oil. Separable by careful chromatography into diastereoisomers.

S-*Dioxide:* [78656-83-4]. *1-Methylene-2-(phenylsulfonyl)cyclopropane. 1-Methylidene-2-(phenylsulfonyl)cyclopropane. [(Methylenecyclopropyl)sulfonyl]benzene, 9CI*
$C_{10}H_{10}O_2S$ M 194.254
Cryst. Mp 47.5-48.5°.

Weber, A. *et al*, *Helv. Chim. Acta*, 1988, **71**, 2026 (*synth, ir, pmr, ms*)

2-Methylheneicosane, 9CI M-80091

$$H_3C(CH_2)_{18}CH(CH_3)_2$$

$C_{22}H_{46}$ M 310.605
Found in orange oil (*Citrus sinensis*) and hops (*Humulus lupulus*).

Steibl, M. *et al*, *Collect. Czech. Chem. Commun.*, 1964, **29**, 2522 (*synth*)
Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al*, *Phytochemistry*, 1966, **5**, 807 (*isol*)

3-Methylheptacosane, 9CI M-80092

[14167-66-9]

$$H_3C(CH_2)_{23}CH(CH_3)CH_2CH_3$$

$C_{28}H_{58}$ M 394.766
Isol. from tobacco (*Nicotiana tabacum*) hop oil (*Humulus lupulus*) orange oil (*Citrus sinensis*), and insect cuticle. n_D^{50} 1.4407.

[55194-24-6]

Mold, J.D. *et al*, *Biochemistry*, 1963, **2**, 605 (*isol*)
Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al*, *Phytochemistry*, 1966, **5**, 807 (*isol*)

3-Methyl-4-hepten-2-one M-80093

[75343-95-2]

$$H_3CCH_2CH{=}CHCH(CH_3)COCH_3$$

$C_8H_{14}O$ M 126.198

Dana, G. *et al*, *Can. J. Chem.*, 1980, **58**, 1451 (*synth, ir, pmr*)
Sato, T. *et al*, *J. Org. Chem.*, 1988, **53**, 1894 (*synth, ms, pmr*)

6-Methyl-6-hepten-2-one, 9CI M-80094

[10408-15-8]

$$H_2C{=}C(CH_3)CH_2CH_2CH_2COCH_3$$

$C_8H_{14}O$ M 126.198
Isol. from fruit oil of *Litsea citrata*. Liq. d_4^{19} 0.846. Bp_{10} 45°. n_D^{19} 1.4344.

2,4-Dinitrophenylhydrazone: [17123-67-0].
Mp 76-78°.

Dimethylhydrazone: [111285-97-3].
$Bp_{8\text{-}10}$ 60°.

Kappeler, H. *et al*, *Helv. Chim. Acta*, 1954, **37**, 957 (*synth, ir*)
Sood, V.K., *Perfum. Essent. Oil Rec.*, 1966, **57**, 285 (*isol*)
Viola, A. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 3462 (*synth*)
Bartlett, P.A. *et al*, *J. Chem. Educ.*, 1984, **61**, 816 (*synth*)
Trehan, I.R. *et al*, *Indian J. Chem., Sect. B*, 1986, **25**, 1243 (*synth, pmr*)

2-Methylhexacosane, 9CI M-80095

[1561-02-0]

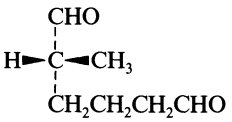
$$H_3C(CH_2)_{23}CH(CH_3)_2$$

$C_{27}H_{56}$ M 380.739
Isol. from hop oil (*Humulus lupulus*), orange oil (*Citrus sinensis*) and insect cuticle.

Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al*, *Phytochemistry*, 1966, **5**, 807 (*isol*)
Streibl, M. *et al*, *Fette, Seifen, Anstrichm.*, 1968, **70**, 543 (*synth*)

2-Methylhexanedial M-80096

2-Methyladipaldehyde



(*R*)-*form*

$C_7H_{12}O_2$ M 128.171

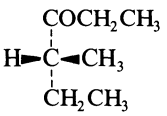
(R)-form [114763-39-2]
Oil.

[114763-40-5]

Hudlicky, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4735 (*synth, ir, pmr*)

4-Methyl-3-hexanone, 9CI M-80097

Updated Entry replacing M-02018
sec-*Butyl ethyl ketone*
[17042-16-9]



(*R*)-*form*

$C_7H_{14}O$ M 114.187

(R)-form [77858-08-3]
Liq. Bp_{100} 74-77°. $[\alpha]_D^{23}$ −30.8° (c, 4 in Et_2O)(96% e.e.).

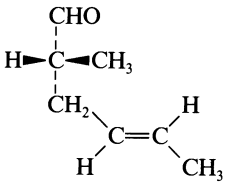
(S)-form [20086-34-4]
$[\alpha]_D^{25}$ +8.5°.

(±)-form
d^{19} 0.825. Bp 134-135°.

Semicarbazone: Mp 137°.

Bartlett, P.D. *et al*, *J. Am. Chem. Soc.*, 1935, **57**, 2580 (*synth, abs config*)
Hudson, B.E. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 3163 (*synth*)
Lardicci, L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 381 (*ord, cd*)
Brown, H.C. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1529 (*synth, pmr, cmr, ir*)

2-Methyl-4-hexenal, 9CI M-80098



$C_7H_{12}O$ M 112.171

(R,E)-form [104372-54-5]

Liq. Bp_{46} 60° (kugelrohr) . Racemises on heating >70°.

Evans, D.A. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 6757 (*synth, pmr*)
Deyo, D.T. *et al*, *Synthesis*, 1988, 608 (*synth, pmr*)

5-Methyl-4-hexen-1-amine M-80099

6-Amino-2-methyl-2-hexene

[115610-15-6]

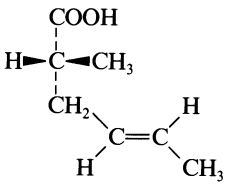
$(H_3C)_2C{=}CHCH_2CH_2CH_2NH_2$

$C_7H_{15}N$ M 113.202

Bp_{20} 51-53°.

Tietze, L.F. *et al*, *Chem. Ber.*, 1989, **122**, 997 (*synth, pmr, cmr*)

2-Methyl-4-hexenoic acid M-80100



(R,E)-form

$C_7H_{12}O_2$ M 128.171

(R,E)-form [93553-73-2]

$[\alpha]_D^{20}$ −10.2° (c, 1.2 in C_6H_6).

(±-E)-form [118492-11-8]

Yellow oil.

Et ester: [118942-48-6].

$C_9H_{16}O_2$ M 156.224

Oil. Bp_{18} 70-75°.

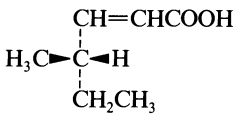
Deyo, D.T. *et al*, *Synthesis*, 1988, 608 (*synth, pmr, ir*)

4-Methyl-2-hexenoic acid, 9CI M-80101

Updated Entry replacing M-02032

4-Ethyl-4-methylcrotonic acid

[37549-83-0]



S-form

$C_7H_{12}O_2$ M 128.171

(S,E)-form [82166-24-3]

Prod. of hydrolysis of Leucinostatin A. $[\alpha]_D^{20}$ +49.7° (c, 0.25 in $CHCl_3$).

Me ester:

$C_8H_{14}O_2$ M 142.197

Liq. Bp_{14} 70°. $[\alpha]_D^{20}$ +37° (c, 0.4 in CH_2Cl_2).

(±)-form

Bp_{13} 125°. $n_D^{20.3}$ 1.4526.

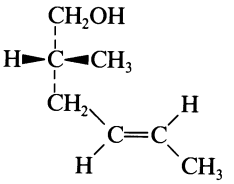
Chloride:

$C_7H_{11}ClO$ M 146.616

Bp_{11} 65-66°.

Linstead, R.P. *et al*, *J. Chem. Soc.*, 1930, 2072 (*synth*)
Mori, Y. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 94 (*isol, ir, pmr*)
Baker, R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 85 (*ester, ir, pmr, ms*)

2-Methyl-4-hexen-1-ol M-80102



(R,E)-form

$C_7H_{14}O$ M 114.187

(R,E)-form

Oil. Bp_{20} 85° (Kugelrohr) . $[\alpha]_D$ +2.5° (c, 1.08 in CH_2Cl_2).

(±)-(E)-form [58927-95-0]

Characterised spectroscopically.

(±)-(Z)-form [58927-94-9]

Characterised spectroscopically.

Chantegnel, B. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2639 (*synth, ir*)
Evans, D.A. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 6757 (*synth, ir, pmr, cmr*)
Deyo, D.T. *et al*, *Synthesis*, 1988, 608 (*synth, pmr, cmr*)

2-Methyl-4-hexen-2-ol, 9CI M-80103

[70910-33-7]

$(H_3C)_2C(OH)CH_2CH{=}CHCH_3$

$C_7H_{14}O$ M 114.187

Bp_{747} 139-140°.

(E)-form [19639-97-5]

n_D^{20} 1.4321.

(Z)-form [19639-96-4]

n_D^{20} 1.4370.

Zurquiyah, A. *et al*, *J. Org. Chem.*, 1969, **34**, 1504 (*synth*)
Hosomi, A. *et al*, *Tetrahedron Lett.*, 1976, 1295 (*synth*)
Lupton, M.F. *et al*, *J. Org. Chem.*, 1978, **43**, 1409 (*synth*)
Fujita, K. *et al*, *Chem. Lett.*, 1982, 1819 (*synth*)
Satoh, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 1791 (*synth, ir, pmr, ms*)

2-Methyl-5-hexen-1-ol, 9CI M-80104

[25913-88-6]

$H_2C{=}CHCH_2CH_2CH(CH_3)CH_2OH$

$C_7H_{14}O$ M 114.187

(±)-form

Odorous liq. d_4^{20} 0.843. Bp_{736} 166-168°, Bp_{25} 88°. n_D^{22} = 1.438.

Allophanate: Cryst. (EtOH). Mp 136°.

Ac:

$C_9H_{16}O_2$ M 156.224

Liq. Bp_{747} 182-184°. n_D^{22} 1.425.

Me ether: 6-Methoxy-5-methyl-1-hexene

$C_8H_{16}O$ M 128.214

Liq. d_4^{25} 0.875. Bp_{20} 76°. n_D^{25} 1.425.

Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 177 (*synth*)
Brettle, R. *et al*, *J. Chem. Soc.*, 1962, 4836 (*synth, uv*)
Brown, H.C. *et al*, *J. Org. Chem.*, 1983, **48**, 644 (*synth, pmr, cmr*)

3-Methyl-5-hexen-1-ol, 9CI M-80105

[25913-87-5]

$H_2C{=}CHCH_2CH(CH_3)CH_2CH_2OH$

$C_7H_{14}O$ M 114.187

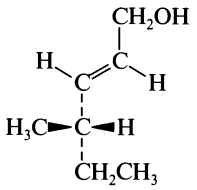
(±)-*form*

Liq. Bp 160°, Bp_{18} 77°. n_D^{20} = 1.4407.

α-*Naphthylurethane:* Cryst. (pet. ether). Mp 45-46°.

Closson, W.D. *et al*, *J. Org. Chem.*, 1970, **35**, 3737 (*synth, pmr*)
Courtois, G. *et al*, *J. Organomet. Chem.*, 1973, **52**, 241 (*synth, ir, raman*)
Beckwith, A.L.J. *et al*, *Aust. J. Chem.*, 1983, **36**, 545 (*synth, pmr*)
Carr, S.A. *et al*, *J. Org. Chem.*, 1985, **50**, 2782 (*synth*)

4-Methyl-2-hexen-1-ol, 9CI M-80106



(*S,E*)-*form*

$C_7H_{14}O$ M 114.187

(*S,E*)-*form* [103064-73-9]

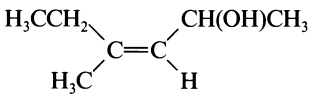
Bp_{14} 90°. $[\alpha]_D^{20}$ +35.2°.

(±)-(*E*)-*form* [87219-85-0]

Liq.

Miller, B.R. *et al*, *Tetrahedron Lett.*, 1983, **24**, 2055 (*synth*)
Hanessian, S. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2776 (*synth*)
Baker, R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 85 (*synth, uv, pmr, ms*)

4-Methyl-3-hexen-2-ol, 9CI M-80107



$C_7H_{14}O$ M 114.187

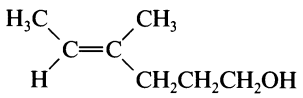
(±)-(*Z*)-*form* [42998-32-3]

Liq. Bp_{35} 76-78°. n_D^{20} = 1.4437.

Normant, J.F. *et al*, *J. Organomet. Chem.*, 1974, **77**, 269 (*synth, ir, raman*)

4-Methyl-4-hexen-1-ol, 9CI M-80108

[59518-07-9]



(*E*)-*form*

$C_7H_{14}O$ M 114.187

(*E*)-*form* [57253-27-7]

Bp_{12} 79°. n_D^{20} 1.4500 (1.4520).

α-*Naphthylurethane:* Plates (pet. ether). Mp 75.5-76.5°.

(*Z*)-*form* [57253-26-6]

Bp_{15} 82-83°. n_D^{20} = 1.4499.

α-*Naphthylurethane:* Cryst. (pet. ether). Mp 65-67° (61-65°).

Diphenylurethane: Laths (pet. ether). Mp 99.5-101° (93-95°).

Ansell, M.F. *et al*, *J. Chem. Soc.*, 1958, 3388 (*synth, ir*)
Julia, M. *et al*, *Tetrahedron*, 1975, **31**, 1737 (*synth, ir, raman*)
Hartmann, J. *et al*, *Helv. Chim. Acta*, 1976, **59**, 453 (*synth, ms, ir, pmr*)
Depezay, J.C. *et al*, *Bull. Soc. Chim. Fr.*, (*Part II*), 1981, 435 (*synth, ir, raman, ms*)

4-Methyl-4-hexen-2-ol, 9CI M-80109

$H_3CCH{=}C(CH_3)CH_2CH(OH)CH_3$

$C_7H_{14}O$ M 114.187

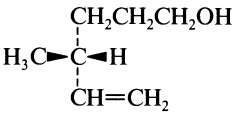
Liq. $Bp_{0.1}$ 28-30°. Mixt. of (*E*)- and (*Z*)-forms.

[108686-09-5, 108686-15-3]

Barluenga, J. *et al*, *Synthesis*, 1987, 318 (*synth, ir, pmr, ms, cmr*)

4-Methyl-5-hexen-1-ol, 9CI M-80110

[25906-56-3]



(*R*)-*form*

$C_7H_{14}O$ M 114.187

(*R*)-*form* [69274-97-1]

Bp_{25} 79-81°. $[\alpha]_D^{19}$ −15.5° (neat). n_D^{19} 1.4371.

(±)-*form*

Liq. Bp_{12} 68°. n_D^{22} 1.4375.

α-*Naphthylurethane:* Cryst. (pet. ether). Mp 55.5-56.0°.

[69274-92-6]

Closson, W.D. *et al*, *J. Org. Chem.*, 1970, **35**, 3737 (*synth, pmr*)
Mori, K. *et al*, *Tetrahedron Lett.*, 1978, **37**, 3447 (*synth*)
Naef, F. *et al*, *Helv. Chim. Acta*, 1981, **64**, 1387 (*synth, pmr, ms*)
Utimoto, K. *et al*, *Heterocycles*, (*Spec. issue*), 1982, **18**, 149 (*synth, uv, pmr, ms*)
Beckwith, A.L.J. *et al*, *Aust. J. Chem.*, 1983, **36**, 545 (*synth, pmr*)
Carr, S.A. *et al*, *J. Org. Chem.*, 1985, **50**, 2782 (*synth, cmr*)

5-Methyl-4-hexen-2-ol, 9CI M-80111

[3695-33-8]

$(H_3C)_2C{=}CHCH_2CH(OH)CH_3$

$C_7H_{14}O$ M 114.187

Baker, R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 727 (*synth*)

5-Methyl-4-hexen-3-ol, 9CI M-80112

[53555-59-2]

$(H_3C)_2C{=}CHCH(OH)CH_2CH_3$

$C_7H_{14}O$ M 114.187

Intermed. for Chrysanthemic acid.

(±)-*form*

Pleasant smelling liq. d_4^{25} 0.837. Bp_{22} 63-65°. n_D^{25} 1.4380.

Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1956, 188 (*synth*)
Deno, N.C. *et al*, *J. Org. Chem.*, 1975, **40**, 514 (*synth, pmr*)
Japan. Pat., 76 86 410, (1976); *CA*, **86**, 120799q (*synth, use*)
Kondo, K. *et al*, *Tetrahedron Lett.*, 1976, **48**, 4359 (*use*)

5-Methyl-5-hexen-1-ol, 9CI M-80113

[5212-80-6]

$H_2C{=}C(CH_3)CH_2CH_2CH_2CH_2OH$

$C_7H_{14}O$ M 114.187

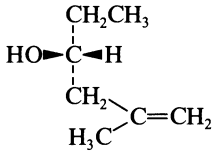
Liq. d_4^{20} 0.845. Bp_{12} 80-82°. n_D^{20} 1.4470 (1.4415).

Phenylurethane: Mp 52-53°.

Eschenmoser, A. *et al*, *Helv. Chim. Acta*, 1952, **35**, 1660 (*synth, ir*)
Zweifel, G. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 190 (*synth, ir*)

Sato, F. *et al*, *J. Organomet. Chem.*, 1977, **142**, 71 (*synth, pmr*)
Sato, F. *et al*, *Chem. Lett.*, 1978, 999 (*synth*)
Carr, S.A. *et al*, *J. Org. Chem.*, 1985, **50**, 2782 (*synth, cmr*)
Gardette, M. *et al*, *Tetrahedron*, 1985, **41**, 5887 (*synth, pmr, cmr*)

5-Methyl-5-hexen-3-ol, 9CI M-80114



(*R*)-*form*

$C_7H_{14}O$ M 114.187

(***R***)-***form*** [77118-89-9]
$[\alpha]_D^{20}$ +5.13° (c, 3.51 in Et_2O).

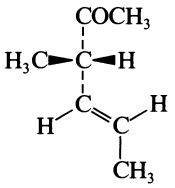
(***S***)-***form*** [67760-89-8]
Bp_{60} 78-80°. $[\alpha]_D^{23}$ −3.07° (neat).

(±)-***form***
Sharp smelling liq. d_4^{22} 0.836. Bp_{30} 63°. n_D^{20} 1.4384.

Herold, T. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1978, **17**, 768 (*synth*)
Hoffmann, R.W. *et al*, *Chem. Ber.*, 1981, **114**, 375 (*synth, pmr*)
Brown, H.C. *et al*, *Tetrahedron Lett.*, 1984, **25**, 5111 (*synth*)
Jadhev, P.K. *et al*, *J. Org. Chem.*, 1986, **51**, 432 (*synth*)

3-Methyl-4-hexen-2-one M-80115

[72189-24-3]



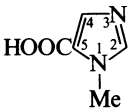
$C_7H_{12}O$ M 112.171

(***S,E***)-***form*** [101223-88-5]
$[\alpha]_D^{20}$ +282°.

Bartik, T. *et al*, *J. Organomet. Chem.*, 1985, **291**, 253 (*synth*)
Sato, T. *et al*, *J. Org. Chem.*, 1988, **53**, 1894 (*synth, pmr, ir, ms*)

1-Methyl-1*H*-imidazole-5-carboxylic acid, 9CI M-80116

Updated Entry replacing M-02077
3-Methyl-4-imidazolecarboxylic acid
[41806-40-0]



$C_5H_6N_2O_2$ M 126.115
Mp 256-257° (245-248°) dec.

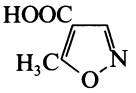
Picrate: Leaflets (H_2O). Spar. sol. H_2O, EtOH. Mp 198-199°.

Me ester:
$C_6H_8N_2O_2$ M 140.141
Prisms (MeOH). Sol. H_2O, EtOH, $CHCl_3$, spar. sol. cold Et_2O. Mp 68-70°.

Hubball, W. *et al*, *J. Chem. Soc.*, 1928, 28 (*synth*)
O'Connell, J.F. *et al*, *Synthesis*, 1988, 767 (*synth, ir, pmr, cmr*)

5-Methyl-4-isoxazolecarboxylic acid M-80117

[42831-50-5]



$C_5H_5NO_3$ M 127.099
Prepn. well descr. but no phys. props. reported.

Et ester: [51135-73-0].
$C_7H_9NO_3$ M 155.153
No phys. props. reported.

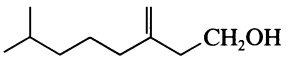
Chloride:
$C_5H_4ClNO_2$ M 145.545
Pungent liq. Bp_{14} 78-79°.
▷ Explosion haz. on dist.

Tamura, Y. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 2580 (*synth*)
Doleschall, G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1875 (*synth, chloride, ir*)

7-Methyl-3-methylene-1-octanol, 9CI M-80118

Bupleurol

[57197-03-2]



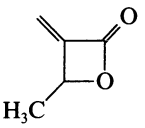
$C_{10}H_{20}O$ M 156.267
Isol. from ethereal oil of *Bupleurum fruticosum* and from *B. linearifolium* seed oils. Bp 209-210°.

[1407-75-6]

Wolinsky, J. *et al*, *J. Org. Chem.*, 1976, **41**, 278 (*synth, ir, pmr*)
Ashraf, M. *et al*, *Pak. J. Sci. Ind. Res.*, 1979, **22**, 325; *ca*, **93**, 245254j (*isol*)

4-Methyl-3-methylene-2-oxetanone M-80119

[117203-16-4]



$C_5H_6O_2$ M 98.101
First α-methylene-β-propionolactone.

(±)-***form***
Pale-yellow liq. with pungent odour. Et and isopropyl analogues also prepd.
▷ Potential carcinogen.

[117203-17-5, 117203-18-6]

Adam, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1988, **27**, 1536 (*synth*)

3-Methyl-1-naphthaldehyde, 8CI M-80120

3-Methyl-1-naphthalenecarboxaldehyde, 9CI. 1-Formyl-3-methylnaphthalene

[63409-02-9]

$C_{12}H_{10}O$ M 170.210

Sydnes, L.K. *et al*, *Tetrahedron*, 1985, **41**, 5205 (*synth, ir, pmr, ms*)
Gupta, R.B. *et al*, *J. Org. Chem.*, 1989, **54**, 1097 (*synth, ir, pmr, cmr*)

5-Methyl-1-naphthaldehyde, 8CI M-80121

5-Methyl-1-naphthalenecarboxaldehyde, 9CI. 1-Formyl-5-methylnaphthalene

[104306-72-1]

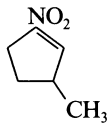
$C_{12}H_{10}O$ M 170.210

2,4-Dinitrophenylhydrazone: Red cryst. Mp 245-246° dec.

Sydnes, L.K. *et al*, *Tetrahedron*, 1985, **41**, 5703 (*synth, ir, pmr, ms*)

3-Methyl-1-nitrocyclopentene M-80122

[112683-42-8]



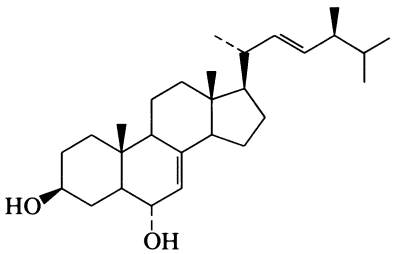
$C_6H_9NO_2$ M 127.143

(±)-form

Liq. $Bp_{0.5}$ 80°.

Denmark, S.E. *et al*, *J. Org. Chem.*, 1988, **53**, 1251 (*synth, pmr, cmr, ms*)

24-Methyl-27-nor-7,22-cholestadiene-3,6-diol M-80123



$C_{27}H_{44}O_2$ M 400.643

(3β,5α,6α,22E)-form

Constit. of *Spongionella gracilis*. Cryst. (MeOH/pet. ether). Mp 185-187°.

Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol, pmr*)

2-Methyloctacosane M-80124

[1560-98-1]

$$H_3C(CH_2)_{25}CH(CH_3)_2$$

$C_{29}H_{60}$ M 408.793

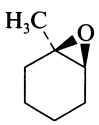
Present in hop, tobacco and orange oil. Found in many insects. Liq.

Mold, J.D. *et al*, *Biochemistry*, 1963, **2**, 605.
Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1670.
Hunter, G.L.K. *et al*, *Phytochemistry*, 1966, **5**, 807.

1-Methyl-7-oxabicyclo[4.1.0]heptane, 9CI M-80125

1-Methylcyclohexene oxide. 1,2-Epoxy-1-methylcyclohexane

[1713-33-3]



(1*R*,2*S*)-*form*

$C_7H_{12}O$ M 112.171

(1R,2S)-form [56246-60-7]

$[\alpha]_D^{25}$ −18-65° (neat).

(1RS,2SR)-form [60363-27-1]

Bp 130-131° (138-142°), Bp_{35} 52°.

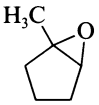
[56246-59-4]

Tani, K. *et al*, *Tetrahedron Lett.*, 1979, 3017 (*synth*)
Curci, R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1984, 155 (*synth*)
Itoi, Y. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 1583 (*synth*)
Robinson, P.L. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 5210 (*synth, cmr*)
De Poorter, B. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1985, 1735 (*synth*)
Yamomoto, H. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1986, 173 (*synth, nmr*)
Robinson, P.L. *et al*, *Phosphorus Sulfur*, 1986, **26**, 15 (*synth*)
Nwaukwa, S.O. *et al*, *Synth. Commun.*, 1986, **16**, 309 (*synth, ir, pmr*)
Davis, F.A. *et al*, *Tetrahedron Lett.*, 1986, **27**, 5079 (*synth*)

1-Methyl-6-oxabicyclo[3.1.0]hexane M-80126

1-Methylcyclopentene oxide. 1,2-Epoxy-1-methylcyclopentane

[16240-42-9]



$C_6H_{10}O$ M 98.144

Bp 110-111°.

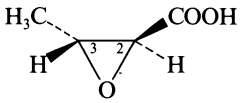
Rebek, J. *et al*, *J. Org. Chem.*, 1979, **44**, 1485 (*synth*)
Johnson, W.S. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 7800 (*synth*)
Blau, K. *et al*, *J. Prakt. Chem.*, 1980, **322**, 915 (*synth, pmr*)
Nwaukura, S.O. *et al*, *Synth. Commun.*, 1986, **16**, 309 (*synth, ir, pmr*)

3-Methyloxiranecarboxylic acid, 9CI M-80127

Updated Entry replacing M-02836

2-Methylglycidic acid. 2,3-Epoxybutyric acid

[2443-40-5]



(2*R*,3*S*)-*form*

$C_4H_6O_3$ M 102.090

(2R,3R)-form

Me ester: $Bp_{1.4}$ 64°. $[\alpha]_D^{22}$ +7.3° (c, 1.26 in $CHCl_3$), $[\alpha]_D^{22}$ −19.0° (c, 1.6 in MeOH).

Et ester: $Bp_{1.5}$ 77°. $[\alpha]_D^{25}$ −1.6° (c, 5.0 in MeOH).

(2S,3S)-form

Me ester: $[\alpha]_D^{22}$ +18.9° (c, 1.8 in MeOH).

Et ester: $[\alpha]_D^{25}$ +1.8° (c, 4.8 in MeOH).

(2R,3S)-form [50468-19-4]

(−)-trans-*form*

Cryst. (C_6H_6). Mp 61°. $[\alpha]_D^{25}$ −82.5° (c, 0.59 in C_6H_6).

Me ester: [50468-20-7].

$C_5H_8O_3$ M 116.116

Liq. Bp 150°.

Et ester:

$C_6H_{10}O_3$ M 130.143

Liq. Bp_{73} 106.5°.

▷ Toxic. ET0875000.

(2S,3R)-form

(+)-trans-*form*

Cryst. Mp 62°. $[\alpha]_D^{20}$ +79° (c, 0.6 in C_6H_6).

(2RS,3SR)-form [13737-02-5]

(±)-trans-*form*

Cryst. (C_6H_6). Mp 84.5-85°.

Me ester: [2980-48-5].

Liq.

Et ester: [19780-35-9].

$C_6H_{10}O_3$ M 130.143

Liq. Bp_{73} 106.5°.

▷ Toxic. ET0875000.

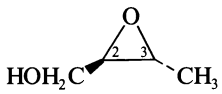
Harada, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1966, **39**, 2311 (*synth, abs config*)
Baldwin, J.E. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 5261 (*synth*)
Aberhart, D.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 7859 (*synth*)
Aberhart, D.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1974, 2320 (*synth*)
Séquin, U., *Tetrahedron Lett.*, 1979, 1833 (*synth, cmr*)
Petit, Y. *et al*, *Synthesis*, 1988, 538 (*synth, ir, pmr*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 663.

3-Methyloxiranemethanol, 9CI M-80128

Updated Entry replacing M-20168

2,3-Epoxy-1-butanol, 8CI. 2-Hydroxymethyl-3-methyloxirane

[872-38-8]



(2*R*,3*R*)-*form*

$C_4H_8O_2$ M 88.106

(2R,3R)-form [58845-50-4]
(+)-trans-*form*
$[\alpha]_D^{25}$ +47° (C_6H_6).

(2S,3S)-form [50468-21-8]
(−)-trans-*form*
$[\alpha]_D$ −49° (c, 5 in C_6H_6).

(2R,3S)-form
(−)-cis-form
Oil. Bp_{15} 64°. $[\alpha]_D^{20}$ −33.6° (c, 0.1 in CH_2Cl_2). 90% enantiomeric excess.

(2S,3R)-form
(+)-cis-form
$[\alpha]_D^{20}$ +29.1° (c, 0.06 in CH_2Cl_2).

(2RS,3RS)-form
(±)-trans-*form*
Bp_{10} 58-59°. n_D^{25} 1.4250.

(2RS,3SR)-form
(±)-cis-*form*
Bp_{10} 69-70°. n_D^{25} 1.4308.

Payne, G.B., *J. Org. Chem.*, 1962, **27**, 3819 (*synth*)
Pierre, J.L. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 4459 (*pmr*)
Aberhart, D.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 7859.
Corey, E.J. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 4618 (*synth*)
Reynolds, K.A. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3195 (*synth, pmr, ms*)

3-Methyl-2-oxobutanoic acid M-80129

Updated Entry replacing M-02849

2-Oxoisopentanoic acid. α-Ketoisovaleric acid. Dimethylpyruvic acid

[759-05-7]

$$(H_3C)_2CHCOCOOH$$

$C_5H_8O_3$ M 116.116
Metab. of *Aspergillus niger* and other microorganisms.
Cryst. Mp 31°. Bp 170.5°.

Oxime: [13010-50-9].
$C_5H_9NO_3$ M 131.131
Cryst. Mp 163-165° dec.

Phenylhydrazone: Long yellow needles (MeOH aq.). Mp 156-157°.

Me ester: [3952-67-8].
$C_6H_{10}O_3$ M 130.143
Bp_{12} 70-80°.

Me ester, 2,4-dinitrophenylhydrazone: Cryst. Mp 176-178°.

Et ester: [20201-24-5].
$C_7H_{12}O_3$ M 144.170
Bp_{10} 58-60°.

Et ester, oxime:
$C_7H_{13}NO_3$ M 159.185
Needles (Et_2O/pet. ether). Mp 57°.

Et ester, semicarbazone: Needles (Et_2O/pet. ether). Mp 95-96°.

Amide: [34906-95-1].
$C_5H_9NO_2$ M 115.132
Mp 106-107°.

Nitrile: [42867-39-0]. *3-Methyl-2-oxobutanenitrile, 9CI. Isobutyryl cyanide*
C_5H_7NO M 97.116
Bp 117-118°.

Moritz, E., *J. Chem. Soc.*, 1881, 13 (*amide*)
Bouveault, L. *et al*, *Bull. Soc. Chim. Fr.*, 1901, 1031 (*synth, derivs*)
Tschelinzeff, W. *et al*, *Chem. Ber.*, 1929, **62**, 2210 (*nitrile*)
Fischer, R. *et al*, *Chem. Ber.*, 1960, **93**, 1387 (*Et ester*)
Zbiral, E. *et al*, *Monatsh. Chem.*, 1966, **97**, 1797 (*Me ester*)
Arfin, S.M., *J. Biol. Chem.*, 1969, **244**, 2250 (*biosynth*)
Clement, B.A. *et al*, *J. Org. Chem.*, 1974, **39**, 97 (*nitrile*)
Cooper, A.J.C. *et al*, *J. Biol. Chem.*, 1975, **250**, 527 (*pmr, bibl*)

6-Methyl-5-oxoheptanoic acid M-80130

[40564-61-2]

$$(H_3C)_2CHCO(CH_2)_3COOH$$

$C_8H_{14}O_3$ M 158.197
$Bp_{0.06}$ 100°.

Et ester: [24071-98-5].
$C_{10}H_{18}O_3$ M 186.250
Bp_{17} 130°.

Iijima, A. *et al*, *Chem. Pharm. Bull.*, 1973, **21**, 215 (*synth*)
Berthelot, P. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1525 (*synth, pmr*)

3-Methylpentacosane, 9CI M-80131

[6902-54-1]

$$H_3C(CH_2)_{21}CH(CH_3)CH_2CH_3$$

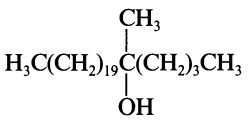
$C_{26}H_{54}$ M 366.713
Isol. from hop oil (*Humulus lupulus*), orange oil (*Citrus sinensis*), and insect cuticle. Liq. Bp_{10} 248°. n_D^{50} 1.4391.

[55194-22-4]

Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al*, *Phytochemistry*, 1966, **5**, 807 (*isol*)
Streibl, M. *et al*, *Fette, Seifen, Anstrichm.*, 1968, **70**, 543; *CA*, **70**, 30318x (*synth*)

5-Methyl-5-pentacosanol, 9CI M-80132

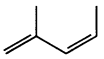
Grandiflorol



$C_{26}H_{54}O$ M 382.712
Isol. from leaves of *Sesbania grandiflora*. Mp 83-84°. $[\alpha]_D$ −20° ($CHCl_3$).

Tiwari, R.D. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1964, **297**, 310.

2-Methyl-1,3-pentadiene M-80133



(*Z*)-*form*

Coml. samples apparently consist mainly of the *Z*-form.

Werstiuk, N.H. *et al*, *Can. J. Chem.*, 1988, **66**, 2954 (*pe*, *config*)

4-Methyl-4-pentenal M-80134

[3973-43-1]

$H_2C{=}C(CH_3)CH_2CH_2CHO$

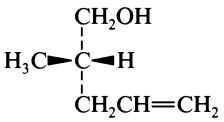
$C_6H_{10}O$ M 98.144
Liq. Bp 99-102°.

2,4-Dinitrophenylhydrazone: Orange cryst. (EtOH). Mp 135-136°.

Vig, O.P. *et al*, *Indian J. Chem.*, 1969, **7**, 1111 (*synth*, *ir*)
Baker, R. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1988, 125 (*synth*)

2-Methyl-4-penten-1-ol M-80135

[5673-98-3]



(*S*)-*form*

$C_6H_{12}O$ M 100.160

(*S*)-*form* [63501-26-8]
d_4^{18} 0.85. Bp 145-146°. $[\alpha]_D$ −2.3° (c, 1.0 in $CHCl_3$).

(±)-*form*
Bp_{12} 57-58°.

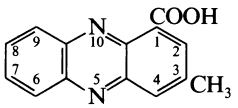
Ac:
$C_8H_{14}O_2$ M 142.197
Bp_{17} 60-65°.

Tetrahydropyranyl ether:
$C_{11}H_{20}O_2$ M 184.278
Bp_3 66-68°.

[17142-57-3, 34288-66-9]

Fray, G.I. *et al*, *J. Chem. Soc.*, 1956, 2036 (*synth*)
Fanta, W.I. *et al*, *J. Org. Chem.*, 1972, **37**, 1624 (*synth*, *ir*, *pmr*, *deriv*)
Evans, D.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2506 (*synth*, *ir*, *pmr*, *cmr*)
Granatica, P. *et al*, *Tetrahedron*, 1988, **44**, 1299 (*synth*)

3-Methyl-1-phenazinecarboxylic acid M-80136



$C_{14}H_{10}N_2O_2$ M 238.245
Mp 212-213°.

Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

4-Methyl-1-phenazinecarboxylic acid, 9CI, 8CI M-80137

[106976-14-1]

$C_{14}H_{10}N_2O_2$ M 238.245
Cryst. (MeOH). Mp 239-241°.

Me ester: [106976-29-8].
$C_{15}H_{12}N_2O_2$ M 252.272
Cryst. (MeOH). Mp 151-152°.

Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843.

6-Methyl-1-phenazinecarboxylic acid, 9CI, 8CI M-80138

[103942-86-5]

$C_{14}H_{10}N_2O_2$ M 238.245
Cryst. (MeOH). Mp 239-241°.

Me ester: [73113-61-8].
$C_{15}H_{12}N_2O_2$ M 252.272
Cryst. (MeOH). Mp 150-151°.

Budzikiewicz, H. *et al*, *J. Heterocycl. Chem.*, 1979, **16**, 1307 (*ester*, *synth*, *uv*, *pmr*, *ms*)
Roemer, A., *Org. Magn. Reson.*, 1982, **19**, 66 (*ester*, *pmr*)
Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

7-Methyl-1-phenazinecarboxylic acid, 9CI, 8CI M-80139

[103942-88-7]

$C_{14}H_{10}N_2O_2$ M 238.245
Cryst. (MeOH). Mp 260° dec.

Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

8-Methyl-1-phenazinecarboxylic acid, 9CI, 8CI M-80140

[106976-15-2]

$C_{14}H_{10}N_2O_2$ M 238.245
Cryst. (MeOH). Mp 238° dec.

Me ester: [83297-74-9].
$C_{15}H_{12}N_2O_2$ M 252.272
Mp 111°.

Budzikiewicz, H. *et al*, *J. Heterocycl. Chem.*, 1979, **16**, 1307 (*ester*, *synth*, *pmr*, *ms*)
Roemer, A., *Org. Magn. Reson.*, 1982, **19**, 66 (*ester*, *pmr*)
Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)
Rewcastle, G.W. *et al*, *Synth. Commun.*, 1987, **17**, 1171 (*synth*)

9-Methyl-1-phenazinecarboxylic acid, 9CI, 8CI M-80141

[58718-46-0]

$C_{14}H_{10}N_2O_2$ M 238.245
Cryst. (MeOH). Mp 237-238°.

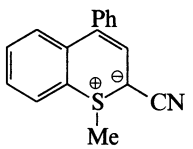
Me ester: [58718-45-9].
$C_{15}H_{12}N_2O_2$ M 252.272
Cryst. (2-propanol). Mp 110-112°.

Breitmaier, E. *et al*, *J. Org. Chem.*, 1976, **41**, 2104 (*synth*, *uv*, *pmr*, *cmr*)
Roemer, A., *Org. Magn. Reson.*, 1982, **19**, 66 (*ester*, *pmr*)
Rewcastle, G.W. *et al*, *J. Med. Chem.*, 1987, **30**, 843 (*synth*)

1-Methyl-4-phenyl-1λ⁴-1-benzothiopyran-2-carbonitrile, 9CI M-80142

2-Cyano-1-methyl-4-phenyl-1-thianaphthalene

[120400-36-4]

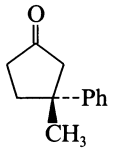


$C_{17}H_{13}NS$ M 263.362

Stable crystalline 1-thianaphthalene. Yellow prisms (CH_2Cl_2/Et_2O). Mp 137-139° dec.

Hori, M. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3816 (*synth, pmr*)

3-Methyl-3-phenylcyclopentanone M-80143



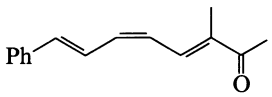
(*R*)-*form*

$C_{12}H_{14}O$ M 174.242

(R)-form [110508-59-3]
Liq. $[\alpha]_D^{26}$ +4.8° (c, 1.02 in $CHCl_3$) (30% e.e.).

Paquette, L.A. *et al*, *J. Org. Chem.*, 1988, **53**, 4978 (*synth, ir, pmr*)

3-Methyl-8-phenyl-3,5,7-octatrien-2-one M-80144



(3*E*,5*Z*,7*E*)-*form*

$C_{15}H_{16}O$ M 212.291

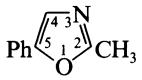
(3E,5Z,7E)-form
Lignarenone A
Metab. of *Scaphander lignarius*.

(3E,5E,7E)-form
Lignarenone B
Isol. from *S. lignarius*.

Cimino, G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 5003.

2-Methyl-5-phenyloxazole, 9CI M-80145

[3969-09-3]



$C_{10}H_9NO$ M 159.187
Mp 58-59°. Bp_{13} 128-130°, Bp_3 101-103°.

Picrate: [14895-06-8].
Mp 155-156°.

Gabriel, S., *Chem. Ber.*, 1910, **43**, 1283 (*synth*)
Houwing, H.A. *et al*, *J. Heterocycl. Chem.*, 1981, **18**, 1133 (*synth, cmr*)

2-Methyl-1-phenyl-2-propen-1-one, 9CI M-80146

α-Methylacrylophenone. 2-Benzoylpropene. Phenyl isopropenyl ketone

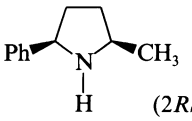
[769-60-8]

$H_2C{=}C(CH_3)COPh$

$C_{10}H_{10}O$ M 146.188
Liq. d_{20}^{20} 1.02. Bp_3 60°.

Burckhalter, J.H. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 4184 (*synth*)
Sugita, K. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1976, **14**, 1901 (*synth, ir, pmr*)
Jackson, L.B. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1791 (*synth, ir, pmr*)

2-Methyl-5-phenylpyrrolidine M-80147



(2*RS*,5*RS*)-*form*

$C_{11}H_{15}N$ M 161.246

(2RS,5RS)-form
(±)-cis-*form*

1-Me: [113579-87-6]. *1,2-Dimethyl-5-phenylpyrrolidine*
$C_{12}H_{17}N$ M 175.273
Oil.

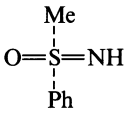
(2RS,5SR)-form
(±)-trans-*form*

1-Me:B,MeI: Needles (Me_2CO/Et_2O). Mp 151-152°.

Tokuda, M. *et al*, *Tetrahedron*, 1987, **43**, 281 (*synth, ir, pmr, cryst struct*)

Methyl phenyl sulfoximine M-80148

Updated Entry replacing M-40125



(*R*)-*form*

(R)-form [60933-65-5]
Low melting solid. Mp 32-34°. $[\alpha]_D^{25}$ −17.9° (c, 2.62 in MeOH).

N-*Me:* [80482-67-3]. N,S-*Dimethyl*-S-*phenylsulfoximine*
$C_8H_{11}NOS$ M 169.247
Reagent for asymmetric synthesis, resoln. and mechanistic studies. Oil. Bp_1 120-125° (bulb) . $[\alpha]_D^{25}$ −135.9° (c, 4.60 in MeOH).

(±)-form [81162-81-4]
Mp 34-35°.

N-*Me:* $Bp_{0.4}$ 115-118°.

N-*Me, picrate:* Mp 189-191°.

[33903-50-3]

Johnson, C.R. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 6594; 1973, **95**, 7418 (*synth*, *N*-Me, pmr, ir, resoln, use)
Oae, S. *et al*, *Int. J. Sulfur Chem., Part A*, 1972, **2**, 491 (*synth*)
Furukawa, N. *et al*, *Synthesis*, 1982, 77 (*synth*)
Shiner, C.S. *et al*, *J. Org. Chem.*, 1988, **53**, 5542 (*synth, resoln, bibl*)

Methylpropanedioic acid, 9CI M-80149

Updated Entry replacing M-03354

Methylmalonic acid. Isosuccinic acid

[516-05-2]

$H_3CCH(COOH)_2$

$C_4H_6O_4$ M 118.089
Needles (EtOAc/pet. ether), prisms (Et_2O/C_6H_6). Sol. EtOH, Et_2O, EtOAc, spar. sol. H_2O, C_6H_6. Mp 135° (120°). pK_a 3.06 (25°).

▷ OO1400000.

Mono-Me ester: [3097-74-3].
$C_5H_8O_4$ M 132.116
Bp_{16} 131°.

Di-Me ester: [609-02-9].
$C_6H_{10}O_4$ M 146.143
d_4^{20} 1.095. Bp 178°.

Dichloride: [39619-07-3].
$C_4H_4Cl_2O_2$ M 154.980
Bp_{50} 75°.

Diamide: [1113-63-9].
$C_4H_8N_2O_2$ M 116.119
Cryst. (H_2O). Insol. Et_2O. Mp 206°.

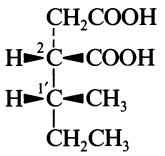
Dianilide: [6833-01-8].
$C_{16}H_{16}N_2O_2$ M 268.315
Leaflets (EtOH). Mp 182° (214°).

Dinitrile: Methylpropanedinitrile, 9CI. Methylmalononitrile.
1,1-*Dicyanoethane*
$C_4H_4N_2$ M 80.089
Needles or oil. Mp 32-34°. Bp_{21} 88-89°.

Meyer, R. *et al, Justus Liebigs Ann. Chem.*, 1906, **347**, 94 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 279 (*synth*)
Aloskalova, N.I. *et al, Zh. Org. Khim.*, 1966, **2**, 2132 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 216.
Hosmane, R.S. *et al, J. Am. Chem. Soc.*, 1982, **104**, 235 (*dinitrile*)
Yokoyama, M. *et al, Synthesis*, 1988, 813 (*synth, dinitrile*)

(1-Methylpropyl)butanedioic acid, 9CI M-80150

Updated Entry replacing M-03392
sec-*Butylsuccinic acid. 3-Methylpentane-1,2-dicarboxylic acid. 3-Carboxy-4-methylhexanoic acid*
[5653-98-5]



(2*S*,1′*R*)-*form*

$C_8H_{14}O_4$ M 174.196

Di-Et ester:
$C_{12}H_{22}O_4$ M 230.303
Liq. $Bp_{0.2}$ 75-76°.

(2*S*,1′*R*)-*form* [54976-96-4]
(3*S*,4*R*)-*form*
Mp 101-102°. $[\alpha]_D$ +27.2° (c, 0.934 in $CHCl_3$).

(2*S*,1′*S*)-*form* [39542-12-6]
(3S,4S)-*form*
Mp 81-82°. $[\alpha]_D$ +30.6° (c, 0.66 in $CHCl_3$).

(2*RS*,1′*RS*)-*form* [55029-18-0]
(3*RS*,4*RS*)-*form*
Cryst. (H_2O). Mp 83-84°.

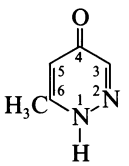
(2*RS*,1′*SR*)-*form* [55029-19-1]
(3RS,4SR)-*form*
Cryst. (H_2O). Mp 135-136°.

[39497-75-1]

Pini, D. *et al, Gazz. Chim. Ital.*, 1974, **104**, 1295.

6-Methyl-4(1*H*)-pyridazinone, 9CI M-80151

6-Methyl-4-pyridazinol. 4-Hydroxy-6-methylpyridazine
[17417-58-2]



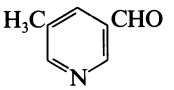
$C_5H_6N_2O$ M 110.115
Needles (EtOH), flakes (H_2O). Mp 238° (231-233°).

[22390-44-9]

Itsuo, I. *et al, Agric. Biol. Chem.*, 1967, **31**, 979 (*synth, uv, pmr*)
Becker, H.G.O. *et al, J. Prakt. Chem.*, 1969, **311**, 286 (*synth, uv, ir*)

5-Methyl-3-pyridinecarboxaldehyde M-80152

5-Methylnicotinaldehyde
[100910-66-5]



C_7H_7NO M 121.138
Low melting solid. Mp 37°. Bp_{20} 130°, $Bp_{0.5}$ 68°.

Semicarbazone: Cryst. (H_2O). Mp 244°.

Phenylhydrazone: Yellow cryst. (MeOH). Mp 145°.

Oxime:
$C_7H_8N_2O$ M 136.153
Cryst. (H_2O). Mp 153°.

Mathes, W. *et al, Chem. Ber.*, 1960, **93**, 286 (*synth, deriv*)
Kyba, E.P. *et al, J. Org. Chem.*, 1988, **53**, 3513 (*synth, pmr, ir*)

5-Methyl-2-pyridinecarboxylic acid, 9CI M-80153

Updated Entry replacing M-03479
5-Methylpicolinic acid
[4434-13-3]

$C_7H_7NO_2$ M 137.138
Cryst. (C_6H_6). Mp 167-168°.

▷ TJ7556000.

1-Oxide: [31283-69-9].
$C_7H_7NO_3$ M 153.137
Cryst. (MeOH). Mp 160-161°.

Me ester: [29681-38-7].
$C_8H_9NO_2$ M 151.165
Cryst. (pet. ether). Mp 54-55°.

Amide: [20970-77-8].
$C_7H_8N_2O$ M 136.153
Mp 178°.

Nitrile: 2-Cyano-5-methylpyridine
$C_7H_6N_2$ M 118.138
Cryst. by subl. Mp 70°.

Ferles, M. *et al, Collect. Czech. Chem. Commun.*, 1968, **33**, 3848 (*synth, amide, nitrile*)
Brzezinski, B. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1970, **18**, 247 (*ir*)
Deady, L.W. *et al, Aust. J. Chem.*, 1971, **24**, 385 (*synth*)
Brezezinski, B. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1973, **47**, 445 (*pmr*)
Deady, L.W. *et al, Org. Magn. Reson.*, 1975, **7**, 41 (*nmr*)
Dormagen, W. *et al, Synthesis*, 1988, 636 (*amide, synth, pmr, cnr*)

5-Methyl-3-pyridinecarboxylic acid, 9CI M-80154

Updated Entry replacing M-03480
5-Methylnicotinic acid. β-Picoline-5-carboxylic acid
[3222-49-9]

$C_7H_7NO_2$ M 137.138
Cryst. (EtOH). Mp 215-216° (208-212°). pK_a 5.2.

Me ester: [29681-45-6].
$C_8H_9NO_2$ M 151.165
Cryst. (hexane). Mp 45-46°.

Amide: [70-57-5].
$C_7H_8N_2O$ M 136.153
Cryst. (EtOAc). Mp 163-165°.

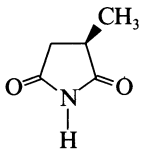
Nitrile: [42885-14-3]. *3-Cyano-5-methylpyridine*
$C_7H_6N_2$ M 118.138
Cryst. (EtOH/pet. ether). Mp 83-84°.

McElvain, S.M. *et al, J. Am. Chem. Soc.*, 1943, **65**, 2233 (*synth*)
Deady, L.W. *et al, Aust. J. Chem.*, 1971, **24**, 385 (*synth*)

Deady, L.W. *et al*, *Org. Magn. Reson.*, 1975, **7**, 41 (*nmr*)
Kyba, E.P. *et al*, *J. Org. Chem.*, 1988, **53**, 3513 (*ester, amide, pmr, ir*)

3-Methyl-2,5-pyrrolidinedione, 9CI M-80155

2-Methylsuccinimide



(*R*)-*form*

$C_5H_7NO_2$ M 113.116

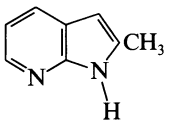
(***R***)-***form*** [117307-07-0]
Cryst. (toluene). Mp 78°. $[\alpha]_D^{20}$ +29.4° (c, 2 in $CHCl_3$).

(±)-***form***
Mp 62°.

Turner, D.W., *J. Chem. Soc.*, 1957, 4555.
Poloński, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 629 (*synth, ir, pmr, cd*)

2-Methyl-1*H*-pyrrolo[2,3-*b*]pyridine M-80156

2-Methyl-7-azaindole
[23612-48-8]

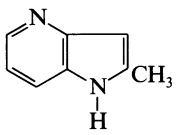


$C_8H_8N_2$ M 132.165
Cryst. (Et_2O). Mp 142° (134-135°).
Picrate: Pale-yellow needles (Me_2CO). Mp 229°.
N-*Benzoyl:*
$C_{15}H_{12}N_2O$ M 236.273
Mp 94-95°.

Clemo, G.R. *et al*, *J. Chem. Soc.*, 1945, 603 (*synth*)
Herbert, R. *et al*, *J. Chem. Soc. C*, 1969, 1505 (*synth, uv, pmr*)
Estel, L. *et al*, *J. Org. Chem.*, 1988, **53**, 2740 (*synth, ir, pmr*)

2-Methyl-1*H*-pyrrolo[3,2-*b*]pyridine M-80157

2-Methyl-4-azaindole

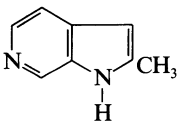


$C_8H_8N_2$ M 132.165
Prisms(C_6H_6). Mp 193-194°.
Picrate: Prisms (Me_2CO). Mp 262° dec.

Clemo, G.R. *et al*, *J. Chem. Soc.*, 1948, 198 (*synth*)

2-Methyl-1*H*-pyrrolo[2,3-*c*]pyridine M-80158

2-Methyl-6-azaindole
[65645-56-9]

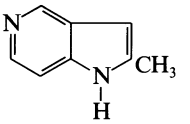


$C_8H_8N_2$ M 132.165
Cryst. by subl. Mp 185°.
B,HCl: Mp 225°.
Picrate: Orange needles. Mp 193°.

Koenigs, E. *et al*, *Ber.*, 1927, **60**, 2106 (*synth*)
Estel, L. *et al*, *J. Org. Chem.*, 1988, **53**, 2740 (*synth, pmr, ir*)

2-Methyl-1*H*-pyrrolo[3,2-*c*]pyridine M-80159

2-Methyl-5-azaindole
[113975-37-4]

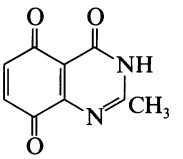


$C_8H_8N_2$ M 132.165
Cryst. by subl. Mp 210°.
Picrate: Bright yellow needles. Mp 213-214° (sinters at 210°).

Clemo, G.R. *et al*, *J. Chem. Soc.*, 1948, 198 (*synth*)
Estel, L. *et al*, *J. Org. Chem.*, 1988, **53**, 2740 (*synth, pmr, ir*)

2-Methyl-4,5,8-quinazolinetrione M-80160

[117498-11-0]

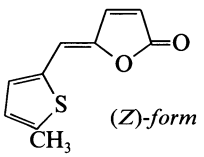


$C_9H_6N_2O_3$ M 190.158
Cryst. Mp 165-168° dec.

Lemus, R.H. *et al*, *J. Org. Chem.*, 1988, **53**, 6099 (*synth, ir, pmr*)

5-[(5-Methyl-2-thienyl)methylene]-2(5*H*)-furanone, 9CI M-80161

5-(5-Methyl-2-thienyl)-2,4-pentadien-4-olide



(*Z*)-*form*

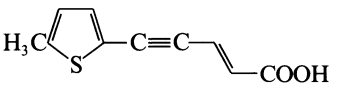
$C_{10}H_8O_2S$ M 192.238

(***E***)-***form*** [35304-91-7]
Needles. Mp 105° approx. Appears to isomerise on heating.

(***Z***)-***form*** [5705-62-4]
Minor constit. of the roots of *Chamaemelum nobile*. Yellow cryst. (pet. ether). Mp 117° (113-115°).

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 1226 (*isol, uv, ir, pmr, struct, synth*)
Yamada, K. *et al*, *Tetrahedron*, 1971, **27**, 5445 (*synth, uv, pmr*)

5-(5-Methyl-2-thienyl)-2-penten-4-ynoic acid M-80162



(*E*)-*form*

$C_{10}H_8O_2S$ M 192.238

(***E***)-***form***
Me ester: Yellowish cryst. (pet. ether). Mp 49°.

(Z)-form [23050-78-4]

Me ester:

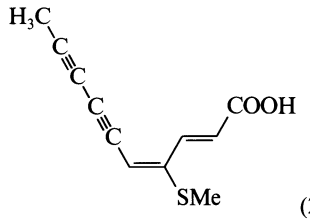
$C_{11}H_{10}O_2S$ M 206.265

Isol. from roots of *Artemisia vulgaris*, *Anthemis nobilis* and *Anacyclus radiatus*. Light-yellow oil. λ_{max} 338 mm (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 1733; 1963, **96**, 584, 588 (*isol*, *uv*, *ir*, *struct*, *synth*)

Schulte, K.E., *Phytochemistry*, 1966, **5**, 949 (*biosynth*)

4-Methylthio-2,4-decadiene-6,8-diynoic acid M-80163



(2*E*,4*E*)-*form*

$C_{11}H_{10}O_2S$ M 206.265

(2E,4E)-form

trans,cis-*form*

Me ester: [13030-72-3].

$C_{12}H_{12}O_2S$ M 220.292

Constit. of roots of *Anthemis tinctoria* and *A. cretica*. Yellow cryst. (Et_2O/pet. ether). Mp 112°.

(2Z,4Z)-form

cis,trans-*form*

Me ester: [13030-70-1].

Isol. from roots of *A. tinctoria*. Yellow needles (pet. ether). Mp 70.5°.

(2Z,4E)-form

cis,cis-*form*

Me ester: [13030-69-8].

Isol. from roots of *A. tinctoria*. Amorph.

(2E,4Z)-form

trans,trans-*form*

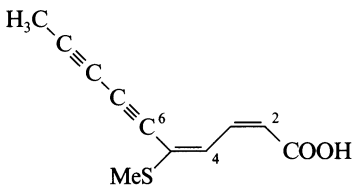
Me ester: [13030-68-7].

Not obt. naturally. Mp 75°.

[57110-47-1, 57110-48-2, 77915-50-5]

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2096; 1968, **101**, 2506; 1975, **108**, 1902 (*isol*, *uv*, *ir*, *struct*, *synth*)

5-Methylthio-2,4-decadiene-6,8-diynoic acid M-80164



(2*Z*,4*E*)-*form*

$C_{11}H_{10}O_2S$ M 206.265

(2Z,4E)-form

cis,cis-*form*

Me ester:

$C_{12}H_{12}O_2S$ M 220.292

Isol. from roots of *Anthemis carpatica*, *A. ruthenica* and other *A.* sp. Light yellow needles (pet. ether). Mp 40°.

Me ester, S-dioxide: Needles (Et_2O/pet. ether). Mp 96°.

6,7-(Z)-dihydro, Me ester: 5-Methylthio-2Z,4E,6Z-decatetrien-8-ynoic acid methyl ester

$C_{12}H_{14}O_2S$ M 222.307

Isol. from roots of *Anthemis tinctoria* and other *A.* sp. Liq. $Bp_{0.001}$ 120°.

(2Z,4Z)-form

cis,trans-*form*

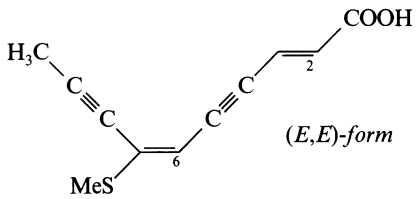
Me ester: Isol. from roots of *A. ruthenica*.

Me ester, S-dioxide: Cryst. ($CHCl_3$). Mp 86°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 1485; 1965, **98**, 1616; 1966, **99**, 2096 (*isol*, *uv*, *ir*, *pmr*, *struct*)

7-Methylthio-2,6-decadiene-4,8-diynoic acid M-80165

[17159-29-4]



(*E*,*E*)-*form*

$C_{11}H_{10}O_2S$ M 206.265

(E,E)-form

trans,cis-*form*

Me ester: [2908-10-3].

$C_{12}H_{12}O_2S$ M 220.292

Isol. from roots of *Anthemis* spp. Yellow cryst. (pet. ether). Mp 46°.

(2E,6Z)-form

cis,cis-*form*

Me ester: Isol. from roots of *A. fuscata*.

Me ester, S-*dioxide:* Mp 99°.

(2Z,6E)-form

cis,cis-*form*

Me ester: [3102-40-7].

Isol. from roots of *A. brachycentros*, *A. tinctoria* and *A. ruthenica*.

Me ester, S-*dioxide:* Cryst. (Et_2O/pet. ether). Mp 58°.

(2Z,6Z)-form

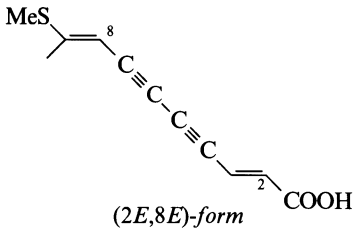
cis,trans-*form*

Me ester: Isol. from various *A.* spp.

Me ester, S-*dioxide:* Cryst. (Et_2O/pet. ether). Mp 65°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 1320; 1963, **96**, 1485; 1965, **98**, 1616; 1966, **99**, 2096 (*isol*, *uv*, *ir*, *pmr*, *struct*)

9-Methylthio-2,8-decadiene-4,6-diynoic acid M-80167



(2*E*,8*E*)-*form*

$C_{11}H_{10}O_2S$ M 206.265

(2E,8E)-form
trans,cis-*form*

Me ester:
$C_{12}H_{12}O_2S$ M 220.292
Isol. from *Anthemis tinctoria*. Cryst. (Et_2O/pet. ether). Mp 75°.

Me ester, S-dioxide: Cryst. (Et_2O/pet. ether). Mp 119-120°.

(2Z,8E)-form
cis,cis-*form*

Me ester: Isol. from roots of *A. tinctoria*, *A. nigrescens* and *A. helwegii*. Cryst. (Et_2O/pet. ether). Mp 40.5°.

Me ester, S-dioxide: Cryst. (Et_2O/pet. ether). Mp 89.5°.

(2E,8Z)-form
trans,trans-*form*

Me ester: Isol. from *A. tinctoria*. Cryst. (Et_2O/pet. ether). Mp 43°.

Me ester, S-dioxide: Cryst. (Et_2O/pet. ether). Mp 101°.

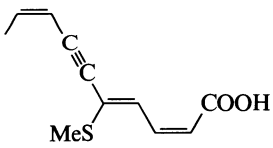
(2Z,8Z)-form
cis,trans-*form*

Me ester: Isol. from *A. tinctoria* and roots of *A. triumfettii*. Cryst. (Et_2O/pet. ether). Mp 41°.

Me ether, S-dioxide: Cryst. (Et_2O/pet. ether). Mp 129.5°.

Bohlmann, E. *et al*, *Chem. Ber.*, 1963, **96**, 1485; 1965, **98**, 1616, 1736; 1966, **99**, 2096 (*isol, uv, ir, pmr, synth, biosynth*)

5-Methylthio-2,4,8-decatrien-6-ynoic acid M-80168



(2*Z*,4*Z*,8*Z*)-*form*

$C_{11}H_{12}O_2S$ M 208.281

(2Z,4Z,8Z)-form
cis, trans, cis-*form*

Me ester: [13103-21-4].
$C_{12}H_{14}O_2S$ M 222.307
Isol. from roots of *Anthemis austriaca*.

Me ester, S,S-*dioxide:* Cryst. (Et_2O/pet. ether). Mp 63-64°.

(2Z,4E,8Z)-form
cis,cis,cis-*form*

Me ester: [13103-22-5].
Isol. from roots of *A. austriaca*.

Me ester, S,S-*dioxide:* Oil.

Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1964, **694**, 149 (*isol, struct*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1967, **100**, 1200 (*synth*)

[1-(Methylthio)ethenyl]benzene, 9CI M-80169

α-(Methylthio)styrene. 1-(Methylthio)-1-phenylethylene

[18624-64-1]

$H_2C{=}CPhSMe$

$C_9H_{10}S$ M 150.244
Oil.

Lecadet, D. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1973, 875 (*synth*)
Leger, L. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 657 (*pmr*)
Schaumann, E. *et al*, *Chem. Ber.*, 1988, **121**, 1159.

[2-(Methylthio)ethenyl]benzene, 9CI M-80170

β-(Methylthio)styrene. Methyl styryl sulfide. 1-(Methylthio)-2-phenylethylene

[7715-02-8]

$PhCH{=}CHSMe$

$C_9H_{10}S$ M 150.244

(E)-form [15436-06-3]
Oil. Bp_{35} 140-142°, Bp_{12} 119°. n_D^{20} 1.6400.

S-*Dioxide:* [15436-11-0]. [*2-(Methylsulfonyl)ethenyl]benzene, 9CI. β-(Methylsulfonyl)styrene. Methyl styryl sulfone.* 1-*(Methylsulfonyl)-2-phenylethylene*
$C_9H_{10}O_2S$ M 182.243
Solid. Mp 76-78°.

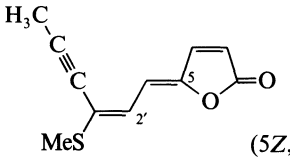
(Z)-form [35822-50-5]
Oil. Bp_{17} 130-140°. n_D^{20} 1.6251.

S-*Dioxide:* [37630-43-6].
Solid. Mp 64.5-66°.

Truce, W.E. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 695 (*synth*)
Wittig, G. *et al*, *Chem. Ber.*, 1961, **94**, 1373 (*synth*)
Caserio, M.C., *J. Am. Chem. Soc.*, 1966, **88**, 5747 (*synth, uv, pmr*)
Bock, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1972, **11**, 150 (*pe*)
Petrov, M.L. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1978, 197 (*synth, ir, pmr*)
Ogura, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 3669 (*synth, ir, pmr*)
Oida, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 959 (*synth, ms*)
Tiecco, M. *et al*, *J. Org. Chem.*, 1983, **48**, 4795 (*synth, deriv*)
Oida, T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1986, 1715 (*synth, pmr*)
Fugami, K. *et al*, *Tetrahedron*, 1988, **44**, 4277 (*synth*)

5-(3-Methylthio-2-hexen-4-ynylidene)-2(5*H*)-furanone M-80171

7-Methylthio-2,4,6-decatrien-8-yn-4-olide



(5*Z*,2′*E*)-*form*

$C_{11}H_{10}O_2S$ M 206.265

(5Z,2′E)-form

trans,cis-*form*

Isol. from roots of *Anthemis kelwayi* and *A. rigescens*. Yellow needles (pet. ether). Mp 67°. Not obt. fully pure.

(5Z, 2′Z)-form

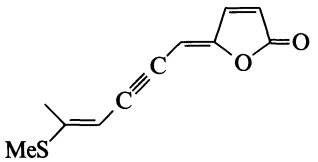
trans,trans-*form*

Isol. from *A. rigescens* and *A. kelwayi*. Yellow platelets (pet. ether). Mp 102°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1616 (*isol, uv, ir, pmr, struct*)

5-(5-Methylthio-4-hexen-2-ynylidene)-2(5*H*)-furanone M-80172

9-Methylthio-2,4,8-decatriene-6-yn-4-olide. 4-Hydroxy-9-(methylthio)-2,4,8-decatrien-6-ynoic acid γ-lactone



$C_{11}H_{10}O_2S$ M 206.265

Isol. from roots of *Anthemis rigescens*.

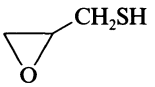
S-Dioxide: Yellowish cryst. (Et_2O). Mp 118.5°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1616; 1966, **99**, 3437 (*isol, uv, ir, pmr, struct, synth*)

(Methylthio)oxirane M-80173

(*Mercaptomethyl*)*oxirane. 1,2-Epoxy-3-mercaptopropane. 2,3-Epoxy-1-propanethiol*

[67757-42-0]



C_3H_6OS M 90.146

(±)-form

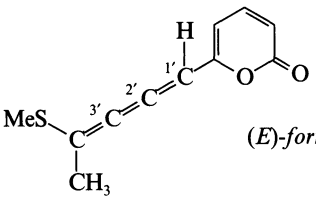
S-*Ph:* [5296-21-9]. [(*Phenylthio*)*methyl*]*oxirane*, *9CI*. 1-*Phenylthio*-2,3-*epoxypropane*

$C_9H_{10}OS$ M 166.243

Oil. $Bp_{0.2}$ 82-85°.

Apparao, S. *et al*, *Synthesis*, 1987, 896 (*synth, pmr*)

6-[4-(Methylthio)-1,2,3-pentatrienyl]-2*H*-pyran-2-one, 9CI M-80174



(*E*)-*form*

$C_{11}H_{10}O_2S$ M 206.265

(E)-form [52061-38-8]

Isol. from fresh roots of *Anthemis austriaca*. Orange-red needles (Et_2O/pet. ether). Mp 108.5-109.5°.

1′,2′-Didehydro, 2′,3′-dihydro (E-): [20903-34-8]. ***6-(4-Methylthio-3-penten-1-ynyl)-2H-pyran-2-one***

Yellow cryst. (CCl_4). Mp 85°.

(Z)-form [20903-32-6]

Isol. from *A. austriaca*. λ_{max} 410 nm.

1′,2′-Didehydro, 2′,3′-dihydro (Z-): [20903-31-5].

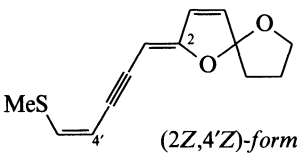
$C_{11}H_{10}O_2S$ M 206.265

Isol. from roots of *A. austriaca*. Yellow cryst. (Et_2O/pet. ether). Mp 68-69°.

Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1966, **694**, 149 (*isol, uv, ir, pmr, ms, struct*)

Bohlmann, F. *et al*, *Chem. Ber.*, 1968, **101**, 3562; 1973, **106**, 3772 (*synth, biosynth*)

2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene, 9CI M-80175



(2*Z*,4′*Z*)-*form*

$C_{13}H_{14}O_2S$ M 234.318

(2Z,4′Z)-form

Isol. from above-ground parts of *Chrysanthemum coronarium*. Oil.

S,S-*Dioxide:* Cryst. (Et_2O). Mp 98.5°. $[\alpha]^{20}_{546}$ −6.1° (c, 3.3 in $CHCl_3$).

(2Z,4′E)-form

Isol. from *C. coronarium*. Yellowish cryst. (pet. ether). Mp 71°. $[\alpha]^{20}_{546}$ +1.2° (c, 7.3 in $CHCl_3$).

S-*Oxide:* ***2-[(5-Methylsulfinyl)-4-penten-2-ynylidene]-1,6-dioxaspiro[4.4]non-3-ene***

$C_{13}H_{14}O_3S$ M 250.318

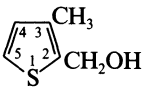
Isol. from *C. coronarium*. λ_{max} 338 nm (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 1179; 1965, **98**, 2605 (*isol, uv, ir, pmr, struct, synth*)

3-Methyl-2-thiophenemethanol, 9CI M-80176

2-Hydroxymethyl-3-methylthiophene

[63826-56-2]



C_6H_8OS M 128.195

Liq. $Bp_{1.5}$ 70-74°. n^{25}_D 1.5524.

α-Naphthylurethane: Glistening plates. Mp 144°.

Campaigne, E. *et al*, *J. Org. Chem.*, 1963, **28**, 914.

4-Methyl-2-thiophenemethanol, 9CI **M-80177**

2-Hydroxymethyl-4-methylthiophene

[74395-18-9]

C_6H_8OS M 128.195

Liq. Bp_1 78-79°. n_D^{20} 1.5512.

Lozanova, A.V. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1980, 958; 1981, 838; *ca*, **93**, 70917y; **95**, 80025m (*synth, ir, uv, pmr*)

5-Methyl-2-thiophenemethanol, 9CI **M-80178**

2-Hydroxymethyl-5-methylthiophene

[63826-59-5]

C_6H_8OS M 128.195

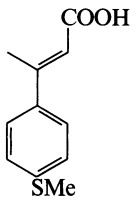
Liq. Bp_3 97-100°. n_D^{20} 1.5090.

Kharchenko, V.G. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1982, 343 (*synth*)

Misharina, T.A. *et al*, *Zh. Anal. Khim.*, 1986, **41**, 1876; *ca*, **106**, 131010h (*ms, glc*)

3-[(4-Methylthio)phenyl]-2-butenoic acid **M-80179**

p-*Methylthio-β-methylcinnamic acid*



$C_{11}H_{12}O_2S$ M 208.281

(E)-form

Me ester:

$C_{12}H_{14}O_2S$ M 222.307

Isol. from roots of *Anthemis tinctoria*.

Me ester, S-*Dioxide:* Cryst. (Et_2O/pet. ether).

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 1834 (*isol, biosynth*)

1-Methylthio-5-phenyl-1-penten-3-yne **M-80180**

[5-(*Methylthio*)-4-*penten-2-ynyl*]*benzene*, *9CI*

$PhCH_2C{\equiv}CCH{=}CHSMe$

$C_{12}H_{12}S$ M 188.293

(Z)-form

Isol. from roots of *Chrysanthemum segetum* and *C. coronarium*. Light-yellow oil. $Bp_{0.1}$ 110°. λ_{max} 274 (ϵ18400), 281 nm (18400)(Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 226; 1964, **97**, 1179 (*isol, uv, ir, pmr, struct*)

5-(Methylthio)-1-phenyl-4-penten-2-yn-1-one, 9CI **M-80181**

1-Methylthio-5-oxo-5-phenyl-1-penten-3-yne

$PhCOC{\equiv}CCH{=}CHSMe$

$C_{12}H_{10}OS$ M 202.276

(E)-form [54668-03-0]

Isol. from roots of *Chrysanthemum segetum*. Oil. λ_{max} 258(ϵ 14400), 336.5 nm (20,000) (Et_2O).

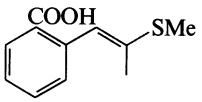
(Z)-form [54668-02-9]

Isol. from roots of *C. segetum* and *C. coronarium*. Cryst. Mp 42.5°. λ_{max} 259(ϵ 15200), 350(13600) nm (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 226, 584; 1964, **97**, 809, 1179 (*isol, uv, ir, pmr, struct, synth, biosynth*)

Mikhelashvili, I.L. *et al*, *Zh. Org. Khim.*, 1974, **10**, 2524 (*synth*)

2-[2-(Methylthio)propenyl]benzoic acid **M-80182**



(*E*)-*form*

$C_{11}H_{12}O_2S$ M 208.281

(E)-form

cis-*form*

Me ester:

$C_{12}H_{14}O_2S$ M 222.307

Isol. from roots of *Anthemis tinctoria*. $Bp_{0.01}$ 64-74°.

Me ester, S-*dioxide:* Cryst. (Et_2O/pet. ether). Mp 62°.

(Z)-form

trans-*form*

Me ester: Isol. from roots of *A. tinctoria*. $Bp_{0.1}$ 81-84°.

Me ester, S-*dioxide:* Cryst. (Et_2O/pet. ether). Mp 77.5-78°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 1485; 1965, **98**, 3087 (*isol, uv, ir, pmr, struct, derivs*)

4-[2-(Methylthio)propenyl]benzoic acid **M-80183**

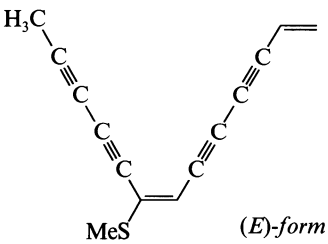
$C_{11}H_{12}O_2S$ M 208.281

Me ester: Isol. from roots of *Anthemis tinctoria*. Cryst. (pet. ether). Mp 54°.

Me ester, S-*dioxide:* Cryst. (Et_2O/pet. ether). Mp 101°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 1485; 1965, **98**, 3087 (*isol, uv, ir, pmr, synth*)

8-Methylthio-1,7-tridecadiene-3,5,9,11-tetrayne **M-80184**



(*E*)-*form*

$C_{14}H_{10}S$ M 210.299

(E)-form

cis-*form*

Isol. from roots of *Flaveria repanda* and *Guzotia abyssinica*. Cryst. (pet. ether). Mp 80° dec.

(Z)-form

trans-*form*

Isol. from roots of *F. repanda* and *G. abyssinica*. Cryst. (Et_2O/pet. ether). Mp 75° dec.

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 1229; 1965, **98**, 876, 3015 (*isol, uv, ir, pmr, biosynth, synth*)

3-Methyltricosane, 9CI **M-80185**

[13410-45-2]

$H_3C(CH_2)_{19}CH(CH_3)CH_2CH_3$

$C_{24}H_{50}$ M 338.659

Isol. from hop oil (*Humulus lupulus*) and orange oil (*Citrus sinensis*) and from insect cuticles. Bp_{10} 233°. n_D^{50} 1.4375.

[55194-20-2]

Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al*, *Phytochemistry*, 1966, **5**, 807 (*isol*)
Streibl,, M. *et al*, *Fette, Seifen, Anstrichm.*, 1968, **70**, 543 (*synth*)

22-Methyl-22-tritetracontanol M-80186

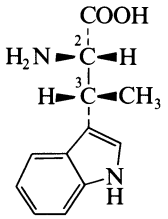
$[H_3C(CH_2)_{20}]_2C(OH)CH_3$

$C_{44}H_{90}O$ M 635.194
Isol. from skin of *Erodium cicutarium*. Mp 65.3-65.6°.

Becker, H.J. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1940, **59**, 933 (*synth*)
van Eijk, J.L., *CA*, 1952, **46**, 9262 (*isol*)

β-Methyltryptophan, 9CI M-80187

Updated Entry replacing M-03847
2-Amino-3-(3-indolyl)butanoic acid



(2*S*,3*R*)-*form*

$C_{12}H_{14}N_2O_2$ M 218.255

(2S,3R)-form
The rel. config. was detd. by Turchin *et al* and the abs. config. follows from the known2*S*-centre present in Telomycin.

(2RS,3RS)-form
Isomer B
Cryst. (H_2O). Mp 247-251° dec.

Me ester:
$C_{13}H_{16}N_2O_2$ M 232.282
Mp 115-118°.

(2RS,3SR)-form
Isomer A
Cryst. (H_2O). Mp 248-250° dec. Cryst. very slowly (several months).

N-*Ac:*
$C_{14}H_{16}N_2O_3$ M 260.292
Cryst. (DMF aq. or EtOH/EtOAc). Mp 216-218°.

Me ester: Mp 121-122°.

Snyder, H.R. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 2217 (*synth*)
Sheehan, J.C. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 2867 (*isol*)
Turchin, K.F. *et al*, *J. Org. Chem.*, USSR (*Engl. transl.*), 1971, **7**, 1329 (*config*)
Behforouz, M. *et al*, *J. Heterocycl. Chem.*, 1989, **25**, 1627 (*synth*)

10-Methylundecanoic acid M-80188

Isododecanoic acid

[2724-56-3]

$(H_3C)_2CH(CH_2)_8COOH$

$C_{12}H_{24}O_2$ M 200.320
Isol. from wool fat, from lipids of *Sarcina lutea* and resin of *Shorea maranti*. Tablets (Me_2CO or C_6H_6). Mp 41.2°. Bp_3 140-145°.

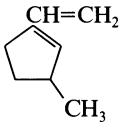
[5129-56-6]

Weitkamp, A.W., *J. Am. Chem. Soc.*, 1945, **67**, 447 (*isol*)
Fieser, L.F. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 3174 (*synth*)
Cocker, W. *et al*, *Perfum. Essent. Oil Rec.*, 1964, **55**, 442 (*isol*)

3-Methyl-1-vinylcyclopentene M-80189

1-Ethenyl-3-methylcyclopentene, 9CI

[114614-93-6]



C_8H_{12} M 108.183

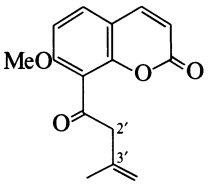
(±)-*form*
Oil.

Fisher, M.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4625 (*synth, pmr, ir, ms*)

Micropubescin M-80190

Updated Entry replacing M-40154

[23560-52-3]



$C_{15}H_{14}O_4$ M 258.273
Constit. of *Micromelum pubescens*. Cryst. Mp 130-131°.

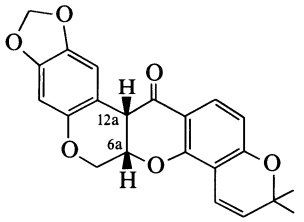
$\Delta^{2',3'}$-*Isomer: 8-(3-Methyl-2-butenoyl)coumarin*
$C_{15}H_{14}O_4$ M 258.273
Constit. of *Ligusticum hultenii*. Mp 131-132°.

Chatterjee, A. *et al*, *Sci. Cult.*, 1967, **33**, 371; 1968, **34**, 366; *CA*, **69**, 2887; **70**, 114946 (*isol*)
Murray, R.D.H. *et al*, *Tetrahedron Lett.*, 1977, 3077 (*synth*)

Millettone M-80191

Updated Entry replacing M-03960

[50376-38-0]



Absolute configuration

$C_{22}H_{18}O_6$ M 378.381

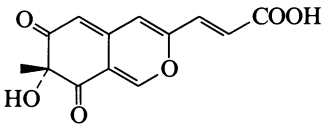
natural-form
Constit. of *Millettia dura*, *Piscida erythrina* and *Lonchocarpus rugosus*. Cream-coloured needles (MeOH). Mp 180-181°. λ_{max} (EtOH) 243 (log ε 4.27), 271 (4.35) and 305 nm (4.10).

6a,12a-*Didehydro:* ***Dehydromillettone***
$C_{22}H_{16}O_6$ M 376.365
Isol. from root of *P. erythrina*. Yellow. Mp 358° dec.

(±)-*form*
Cryst. (C_6H_6/hexane). Mp 245-246°.

Falshaw, C.P. *et al*, *Tetrahedron, Suppl.* 7, 1966, 333 (*isol*)
Ollis, W.D. *et al*, *Tetrahedron*, 1967, **23**, 4741 (*struct, uv, pmr, ord, cd*)
Fujita, F. *et al*, *Agric. Biol. Chem.*, 1973, **37**, 1737 (*synth*)

Mitorubrinic acid M-80192



(*R*)-*form*

$C_{21}H_{16}O_9$ M 412.352

(R)-form

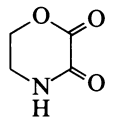
Isol. from *Penicillium funiculosum*. Morphogenic substance inducing chlamydospore-like cells. Yellow cryst. Mp 222-225°. $[\alpha]_D^{22}$ −450° (c, 0.025 in EtOH).

(S)-form [58958-07-9]

Prod. by *Hypoxylon fragiforme*. Yellow microcryst. Mp 225-227° dec. $[\alpha]_D^{25}$ +500° (c, 0.4 in dioxan).

Locci, R. *et al*, *G. Microbiol.*, 1967, **15**, 93 (*isol*)
Chong, R. *et al*, *J. Chem. Soc. C*, 1971, 3571 (*synth*)
Steglich, W. *et al*, *Phytochemistry*, 1974, **13**, 2874 (*isol*)
Natsume, M. *et al*, *Agric. Biol. Chem.*, 1985, **49**, 2517 (*isol, abs config*)

2,3-Morpholinedione M-80193



$C_4H_5NO_3$ M 115.088

N-Et: [73978-21-9].
$C_6H_9NO_3$ M 143.142
Cryst. Mp 70.0-70.5°.

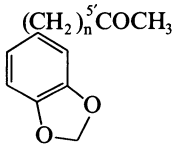
Murahashi, S.I. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 125.

Moskachan B M-80194

Updated Entry replacing M-50261

6-(1,3-Benzodioxol-5-yl)-2-hexanone, 9CI. 6-(3,4-Methylenedioxyphenyl)-2-hexanone

[75787-96-1]



n = 4

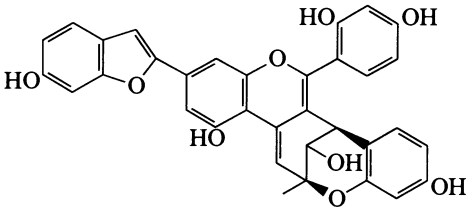
$C_{13}H_{16}O_3$ M 220.268
Constit. of *Ruta angustifolia*. Oil.

5′-Alcohol: [105317-65-5]. ***Moskachan C.*** *6-(3,4-Methylenedioxyphenyl)-2-hexanol*
$C_{13}H_{18}O_3$ M 222.283
From *R. angustifolia*. Oil.

5′-Deoxo, 5′,6′-didehydro: 6-(3,4-Methylenedioxylphenyl)-1-hexene. ***Dehydromoskachan C***
$C_{13}H_{16}O_2$ M 204.268
Constit. of *R. chalepensis* var. *latifolia*. Oil. The name Dehydromoskachan C is misleading.

Borges Del Castillo, J. *et al*, *Phytochemistry*, 1986, **25**, 2209 (*isol*)
Ulubelen, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1012 (*isol*)

Mulberrofuran S M-80195



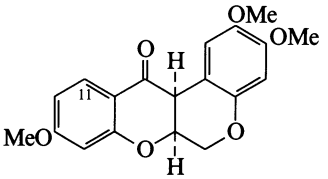
$C_{34}H_{24}O_9$ M 576.558
Isolated from the powder on the surface of *Morus alba* bark. Red amorph. powder. $[\alpha]_D^{23}$ +166° (c, 0.13 in EtOH).

Hano, Y. *et al*, *Heterocycles*, 1989, **28**, 697.

Munduserone M-80196

Updated Entry replacing M-04093

6a,12a-Dihydro-2,3,9-trimethoxy[1]benzopyrano[3,4-b][1]benzopyran-12(6H)-one, 9CI



$C_{19}H_{18}O_6$ M 342.348

(+)-form [3564-85-0]

Constit. of the bark of *Mundulea sericea*. Mp 162°. $[\alpha]_D$ +103° ($CHCl_3$).

11-Hydroxy: [41743-42-4]. ***Sermundone***
$C_{19}H_{18}O_7$ M 358.347
Isol. from root bark of *M. sericea*. Details apparently not publ.

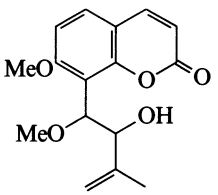
(±)-form [19737-92-9]

Cryst. (C_6H_6/hexane). Mp 171.5-172°.

Finch, N. *et al*, *Proc. Chem. Soc., London*, 1960, 176 (*struct*)
Dyke, S.F. *et al*, *J. Chem. Soc. C*, 1966, 749 (*Sermundone*)
Chandrashekar, V. *et al*, *Tetrahedron*, 1967, **23**, 2505 (*synth*)
Nakatani, N. *et al*, *Agric. Biol. Chem.*, 1968, **32**, 769 (*synth*)
Omokawa, H. *et al*, *Agric. Biol. Chem.*, 1973, **37**, 1717 (*synth*)
Crombie, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 1277 (*synth*)
Amos, P.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 510 (*synth*)

Murracarpin M-80197

[120786-75-6]



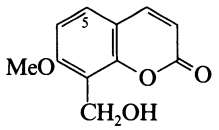
$C_{16}H_{18}O_5$ M 290.315
Constit. of *Murraya paniculata*. Granules (hexane). Mp 164-165°. $[\alpha]_D$ −15.6° (c, 0.068 in $CHCl_3$).

Wu, T.-S. *et al*, *Phytochemistry*, 1989, **28**, 293.

Murrayacarpin A M-80198

8-(Hydroxymethyl)-7-methoxy-2H-1-benzopyran-2-one. 8-Hydroxymethyl-7-methoxycoumarin

[120693-43-8]



$C_{11}H_{10}O_4$ M 206.198

Constit. of *Murraya paniculata*. Needles ($CHCl_3$). Mp 163-166°.

5-Methoxy: [120693-44-9]. *8-(Hydroxymethyl)-5,7-dimethoxy-2H-1-benzopyran-2-one. 8-Hydroxymethyl-5,7-dimethoxycoumarin.* ***Murrayacarpin B***

$C_{12}H_{12}O_5$ M 236.224

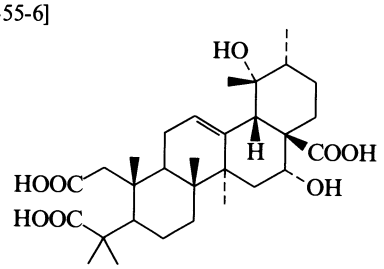
Constit. of *M. paniculata*. Granules ($CHCl_3$). Mp 199-201°.

Wu, T.-S. *et al*, *Phytochemistry*, 1989, **28**, 293.

Musangic acid M-80199

16α,19α-Dihydroxy-2,3-seco-12-ursene-2,3,28-trioic acid, 9CI

[120396-55-6]



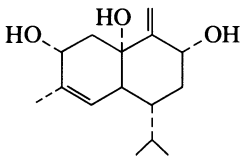
$C_{30}H_{46}O_8$ M 534.689

Constit. of *Musanga cecropioides*.

Lontsi, D. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 52 (*isol, pmr, cmr*)

4,10(14)-Muuroladiene-1,3,9-triol M-80200

1,3,9-Trihydroxymuurolene



$C_{15}H_{24}O_3$ M 252.353

Constit. of *Helichrysum dasyanthum*. Gum.

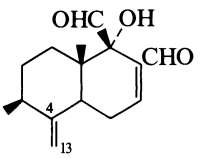
Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1119.

Muzigadial M-80201

Updated Entry replacing M-50280

Canellal

[66550-09-2]



$C_{15}H_{20}O_3$ M 248.321

Isol. from *Warburgia ugandensis* and *Canella winteriana*. Antifeedant. Cryst. Mp 127-128°. $[\alpha]_D^{25}$ −193° (c, 0.2 in $CHCl_3$).

4α,13-Epoxide: ***4α,13-Epoxymuzigadial***

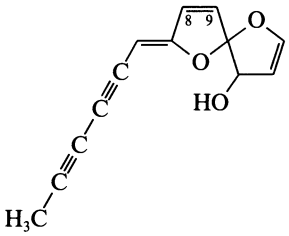
$C_{15}H_{20}O_4$ M 264.321

Constit. of *C. winteriana*. Cryst. (Me_2CO/Et_2O). Mp 140-142°. $[\alpha]_D$ −240° (c, 0.5 in $CHCl_3$).

Kubo, I. *et al*, *Tetrahedron Lett.*, 1977, 4553 (*isol*)
El-Feraly, F.S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 75 (*isol, cryst struct*)
Bosch, M.P. *et al*, *J. Org. Chem.*, 1986, **51**, 773 (*synth*)
Al-Said, M.S. *et al*, *Phytochemistry*, 1989, **28**, 297 (*deriv*)

Mycosinol M-80202

7-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.4]nona-2,8-dien-4-ol, 9CI



$C_{13}H_{10}O_3$ M 214.220

Variable amts. of information on stereochem. of this compd. and its derivs. Isol. from roots of *Chrysanthemum foeniculaceum* and as phytoalexin of *Coleostephus myconis*. Cryst. (Et_2O/pet. ether). Mp 102°. $[\alpha]_D^{20}$ +44° (c, 0.84 in Et_2O).

Ac (E-):

$C_{15}H_{12}O_4$ M 256.257

From *Chrysanthemum lencanthemum, C. segetum, C. coronarium* and *C. ircutianum*. Cryst. (Et_2O/pet. ether). Mp 123°.

Ac (Z-):

$C_{15}H_{12}O_4$ M 256.257

Isol. from *C. leucanthemum, C. segetum, C. coronarium, C. ircutianum* and *C. silvaticum*. Mp 91°.

8,9-Epoxide: ***8,9-Epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-en-4-ol***

$C_{13}H_{10}O_4$ M 230.220

Isol. from above-ground parts of *C. ircutianum*. Cryst. (Et_2O/pet. ether). Mp 139°. $[\alpha]_{546}^{20}$ −145.5° (c, 0.3 in Et_2O).

8,9-Epoxide, Ac: 4-Acetoxy-8,9-epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-ene

$C_{15}H_{12}O_5$ M 272.257

Isol. from *C. leucanthemum* and *C. maximum*. Cryst. (Et_2O/pet. ether). Mp 153.5°. $[\alpha]_{546}^{20}$ −78° (c, 0.88 in Et_2O). A tentative complete stereochem. was assigned to this compd.

6,7-Epoxide, O-angeloyl: 4-Angeloyloxy-8,9-epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-ene

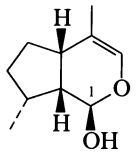
$C_{18}H_{16}O_5$ M 312.321

Isol. from roots of *C. maximum* and above-ground parts of *C. ircutianum*. Cryst. (Et_2O/pet. ether). Mp 133°. $[\alpha]_{546}^{20}$ +47.6° (c, 1.2 in Et_2O).

[111768-19-5]

Bohlmann, F. *et al*, *Chem. Ber.*, 1961, **94**, 3193; 1963, **96**, 226; 1964, **97**, 1179; 1965, **98**, 2596 (*isol, uv, ir, pmr, ord*)
Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1963, **668**, 51 (*config*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1971, **104**, 11 (*ms*)
Zeisberg, R. *et al*, *Chem. Ber.*, 1974, **107**, 3800 (*cmr*)
Marshall, P.S. *et al*, *Phytochemistry*, 1987, **26**, 2493 (*isol*)

3-Myodeserten-1-ol M-80203



(1*R*)-*form*

$C_{10}H_{16}O_2$ M 168.235

(1R)-form

Ac: [95585-89-0]. ***1S-Acetoxy-3-myodesertene***
$C_{12}H_{18}O_3$ M 210.272
Constit. of *Myoporum deserti*. Oil. $[\alpha]_D$ −183° (c, 7.7 in $CHCl_3$).

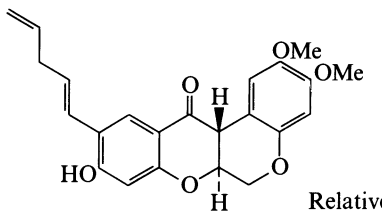
Me ether: [19479-28-8]. ***1-Methoxy-3-myodesertene.***
Myodesertin (obsol.)
$C_{11}H_{18}O_2$ M 182.262
Isol. from *M. deserti*. Bp_2 67°. $[\alpha]_D$ −165° (neat). n_D^{25} 1.4752.

(1S)-form

Ac: [95585-88-9]. ***1R-Acetoxy-3-myodesertene***
$C_{12}H_{18}O_3$ M 210.272
From *M. deserti*. Cryst. (pentane). Mp 17°. $[\alpha]_D$ +273° (c, 2.7 in $CHCl_3$).

Grant, H.G. *et al*, *Aust. J. Chem.*, 1980, **33**, 853; 1985, **38**, 325.

Myriconol M-80204



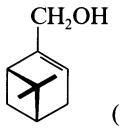
Relative configuration

$C_{23}H_{22}O_6$ M 394.423
Struct. dubious, esp. the side-chain. Isol. from stem bark of *Myrica nagi*. Mp 114°. $[\alpha]_D^{34}$ −60.8° (EtOH).

Krishnamoorthy, V. *et al*, *Curr. Sci.*, 1963, **32**, 16.

Myrtenol M-80205

Updated Entry replacing M-04173
2-Pinen-10-ol. Darwinol
[515-00-4]



(+)-*form*

$C_{10}H_{16}O$ M 152.236

(+)-form [6712-78-3]
Isol. from oil of *Myrtus communis*, *Darwinia grandiflora*, *Leptospermum lanigerum*, *Chamaecyparis formosensis* and others. Oil. Bp_{11} 103-104°. $[\alpha]_D$ +45.5°.

10-Aldehyde: [23727-16-4]. ***Myrtenal***
$C_{10}H_{14}O$ M 150.220
Occurs in eucalyptus and other plant oils. Unstable oil with cinnamon odour. Bp_{15} 99-100°. $[\alpha]_D^{20}$ +14.75°.

10-Carboxylic acid: [601-74-1]. *2-Pinen-10-oic acid. Myrtenic acid*
$C_{10}H_{14}O_2$ M 166.219
Cryst. Mp 53.5-55°. $[\alpha]_D^{20}$ +55° (c, 0.8 in EtOH).

(−)-form

Bp_{11} 101-102°. $[\alpha]_D^{20}$ −47.1° (EtOH).

Ac:
$C_{12}H_{18}O_2$ M 194.273
Isol. from *Valeriana officinalis*.

3-Methylbutanoyl: (−)-*Myrtenyl isovalerate*
Isol. from oil of *V. officinalis*.

10-Aldehyde: [18486-69-6].
Unstable oil. Bp 220-221°. $[\alpha]_D$ −15.3°.

(±)-form
Oil. n_D^{20} 1.4963.

Hydrogen phthalate: Mp 120.5°.

[19250-17-0]

Stoll, A. *et al*, *Helv. Chim. Acta*, 1957, **40**, 1205 (*acetate, isovalerate*)
Couchman, F.M. *et al*, *Tetrahedron*, 1964, **20**, 2037 (*isol*)
Banthorpe, D.V. *et al*, *Chem. Rev.*, 1966, **66**, 643 (*rev*)
Bates, R.B. *et al*, *J. Org. Chem.*, 1968, **33**, 1730 (*pmr*)
Borowiecki, L. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1971, **45**, 573 (*Myrtenic acid*)
Kergomard, A. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 2572 (*synth*)
Rauchschwalbe, G. *et al*, *Helv. Chim. Acta*, 1975, **58**, 1094 (*synth*)
Bohlmann, F. *et al*, *Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)

N

2,3-Naphthalenedicarboxylic acid, 9CI — N-80001

Updated Entry replacing N-60003

[2169-87-1]

$C_{12}H_8O_4$ M 216.193

Prisms (AcOH or by subl.). Sol. hot EtOH, spar. sol. Et_2O. Mp 246°, Mp 239-241°.

Di-Me ester: [13728-34-2].
$C_{14}H_{12}O_2$ M 212.248
Large plates (Et_2O/pet. ether). Mp 47°. Bp_1 141-145°.

Di-Et ester: [50919-54-5].
$C_{16}H_{16}O_2$ M 240.301
Cryst. (Me_2CO). Mp 88.5-89.5°.

Mononitrile: 3-Cyano-2-naphthoic acid
$C_{12}H_7NO_2$ M 197.193
Yellow cryst. Mp 273-274°.

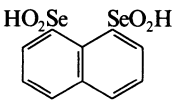
Dinitrile: [22856-30-0]. *2,3-Dicyanonaphthalene*
$C_{12}H_6N_2$ M 178.193
Needles (EtOH). Mp 251°.

*Imide: 2*H*-Naphtho*[2,3-c]*pyrrole*-1,3-*dione*
$C_{12}H_7NO_2$ M 197.193
Microneedles ($CHCl_3$/EtOH). Mp 275°. Softens at 250°.

Anhydride: [716-39-2]. *Naphtho*[*2,3*-c]*furan*-1,3-*dione, 9CI. Naphthalic anhydride*
$C_{12}H_6O_3$ M 198.178
Light yellow cryst. (Me_2CO/pet. ether). Mp 250-252°.

Freund, M. *et al*, *Justus Liebigs Ann. Chem.*, 1913, **402**, 68.
Waldmann, H. *et al*, *Ber.*, 1931, **64**, 1713.
Bradbrook, E.F. *et al*, *J. Chem. Soc.*, 1936, 1739.
Patton, J.W. *et al*, *J. Org. Chem.*, 1965, **30**, 3869.
Cava, M.P. *et al*, *J. Org. Chem.*, 1969, **34**, 538 (*anhydride*)
Davies, C., *Fuel*, 1973, **52**, 270; 1974, **53**, 105 (*ir, uv*)
Org. Synth., Coll. Vol., 5, 1973, 810.
Carlson, R.G. *et al*, *J. Org. Chem.*, 1986, **51**, 3978 (*synth*)
Fier, S. *et al*, *J. Org. Chem.*, 1988, **53**, 2353 (*anhydride*)
Patney, H.K., *J. Org. Chem.*, 1988, **53**, 6106 (*anhydride*)

1,8-Naphthalenediseleninic acid — N-80002



$C_{10}H_8O_4Se_2$ M 350.091

Na salt: Prepd. in soln.

Anhydride: [114031-51-5]. *Naphth*[*1,8*-cd][1,2,6]*oxadiselenin* 1,3-*dioxide*
$C_{10}H_6O_3Se_2$ M 332.076
Solid. Mp 153° dec. Insol. in all common solvents, could not be recryst. nor nmr obtained.

Kice, J.L. *et al*, *J. Org. Chem.*, 1988, **53**, 2435 (*synth, ir, uw*)

1,4,5,7-Naphthalenetetrol, 9CI — N-80003

1,4,5,7-Tetrahydroxynaphthalene

$C_{10}H_8O_4$ M 192.171

5-Me ether, 1,7-Di-Ac: [119098-66-7].
$C_{15}H_{14}O_6$ M 290.272
Cubes (EtOH). Mp 137.5-138.5°.

4,5-Di-Me ether, di-Ac: [119098-67-8].
$C_{16}H_{16}O_6$ M 304.299
Needles (EtOH). Mp 135.5-136°.

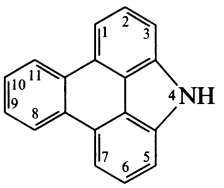
1,4,5-Tri-Me ether, Ac: [119098-76-9].
$C_{15}H_{16}O_5$ M 276.288
Light brown needles (CH_2Cl_2/pet. ether). Mp 75°.

Giles, R.G.F. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2459 (*synth, ir, pmr, ms*)

4*H*-Naphtho[1,2,3,4-*def*]carbazole, 9CI — N-80004

1,12-Iminotriphenylene

[109606-75-9]



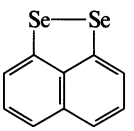
$C_{18}H_{11}N$ M 241.292

Fluffy needles (C_6H_6 or by subl.). Mp 250°. Subl. readily.

Klemm, L.H. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1427 (*synth, uw, pmr, ms*)

Naphtho[1,8-*cd*]-1,2-diselenole — N-80005

[36579-71-2]



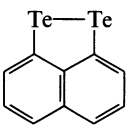
$C_{10}H_6Se_2$ M 284.077

Lustrous purple needles (CH_2Cl_2/hexane). Mp 127-129°.

Meinwald, J. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 255 (*synth, ir, uw, pmr, cmr, ms*)
Kice, J.L. *et al*, *J. Org. Chem.*, 1988, **53**, 2435 (*synth*)

Naphtho[1,8-*cd*]1,2-ditellurole, 9CI — N-80006

[52875-49-7]



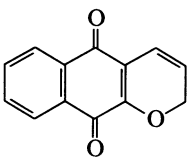
$C_{10}H_6Te_2$ M 381.357

Metallic greenish needles (hexane/CS_2). Mp 212-214°.

Meinwald, J. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 255 (*synth, uw, pmr, cmr, ir, ms*)

2*H*-Naphtho-[2,3-*b*]pyran-5,10-dione — N-80007

[110271-46-0]



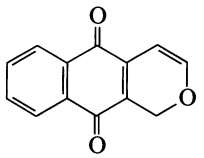
$C_{13}H_8O_3$ M 212.204

Orange prisms. Mp 160-163°.

Hayashi, T. *et al*, *J. Med. Chem.*, 1987, **30**, 2005 (*synth, ir, uv, pmr*)

1*H*-Naphtho[2,3-*c*]pyran-5,10-dione N-80008

[106261-83-0]

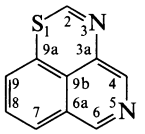


$C_{13}H_8O_3$ M 212.204
Orange cryst.

Hayashi, T. *et al*, *J. Med. Chem.*, 1987, **30**, 2005 (*synth, ir, uv, pmr*)

Naphtho[1,8-*de*]-1,3-thiazine N-80009

[204-07-9]

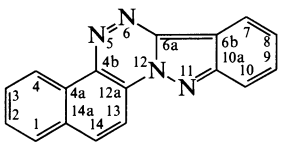


$C_{11}H_7NS$ M 185.249
Green needles melting and resolidifying to prisms. Mp 104-110°, Mp >320° (double Mp).

Herbert, J.M. *et al*, *Heterocycles*, 1987, **26**, 1037 (*synth, pmr*)

Naphtho[2′,1′:5,6][1,2,4]triazino[4,3-*b*]indazole, 9CI N-80010

[221-14-7]



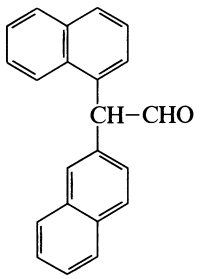
$C_{17}H_{10}N_4$ M 270.293
Orange cryst. (EtOH). Mp 250-251°.

Neidlein, R. *et al*, *Chem. Ber.*, 1988, **121**, 1359 (*synth, ir, uv, pmr, cmr, ms*)

2-(1-Naphthyl)-2-(2-naphthyl)ethanal N-80011

α-2-Naphthalenyl-1-naphthaleneacetaldehyde, 9CI. 2-(α-Naphthyl)-2-(β-naphthyl)acetaldehyde

[91879-84-4]



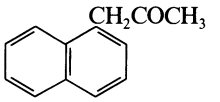
$C_{22}H_{16}O$ M 296.368
Unstable yellow oil.

Zimmerman, H.E. *et al*, *J. Org. Chem.*, 1989, **54**, 2125 (*synth, ir, pmr*)

1-(1-Naphthyl)-2-propanone N-80012

1-(1-Naphthalenyl)-2-propanone. 1-Acetonylnaphthalene. 1-Naphthylacetone

[33744-50-2]



$C_{13}H_{12}O$ M 184.237
Liq. $Bp_{0.75}$ 121-126°, $Bp_{0.4}$ 111-114°.

Oxime (E-): [19534-15-7].
Mp 96-97°.

Semicarbazone: Mp 189.5-190.5°.

[20557-52-2, 85629-15-8]

Kotera, K. *et al*, *Tetrahedron*, 1968, **24**, 5677 (*deriv, synth*)
Zimmerman, H.E. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 3638 (*synth ir, pmr*)
Barcus, R.L. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 3928 (*synth, ir, pmr*)

1-(2-Naphthyl)-2-propanone N-80013

1-(2-Naphthalenyl)-2-propanone, 9CI. 2-Acetonylnaphthalene. 2-Naphthylacetone

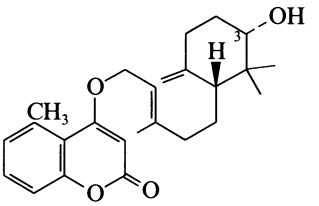
[21567-68-0]

$C_{13}H_{12}O$ M 184.237
Mp 36-37°.

Newman, M.S. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 3342 (*synth*)
Inaba, S. *et al*, *J. Org. Chem.*, 1985, **50**, 1373 (*synth, ir, pmr*)

Nassauvirevolutin A N-80014

[119889-33-7]



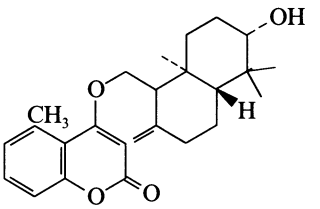
$C_{25}H_{32}O_4$ M 396.525
Constit. of *Nassauvia revoluta*. Gum.

3-Ketone: [119875-28-4]. ***Nassauvirevolutin* B**
$C_{25}H_{30}O_4$ M 394.510
Constit. of *N. revoluta*. Gum.

Bittner, M. *et al*, *Phytochemistry*, 1988, **27**, 3845.

Nassauvirevolutin C N-80015

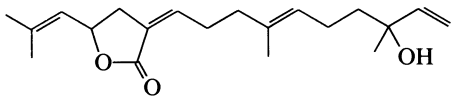
[119875-29-5]



$C_{25}H_{32}O_4$ M 396.525
Constit. of *Nassauvia revoluta*. Gum.

Bittner, M. *et al*, *Phytochemistry*, 1988, **27**, 3845.

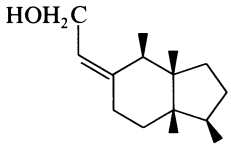
Naviculide N-80016



$C_{20}H_{30}O_3$ M 318.455
Constit. of *Porella navicularis*. Oil.

Toyota, M. *et al*, *Phytochemistry*, 1989, **28**, 1661.

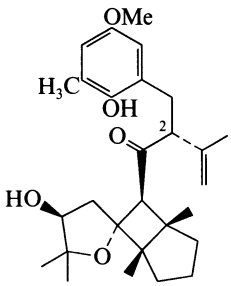
Naviculol N-80017



$C_{15}H_{26}O$ M 222.370
Constit. of *Porella navicularis*. Oil. $[\alpha]_D$ +48.5° (c, 1.14 in $CHCl_3$).

Toyota, M. *et al*, *Phytochemistry*, 1989, **28**, 1661.

Neobalearone N-80018

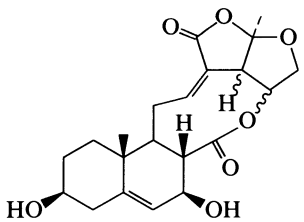


$C_{28}H_{40}O_5$ M 456.621
Metab. of *Cystoseira stricta*. Oil. $[\alpha]_D^{25}$ +120.0° (c, 1.6 in EtOH).

2-Epimer: ***Epineobalearone***
$C_{28}H_{40}O_5$ M 456.621
Metab. of *C. stricta*. Oil. $[\alpha]_D^{25}$ −77.1° (c, 1.86 in EtOH).

Amico, V. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 962 (*isol, pmr, cmr*)

Neocynaponogenin A N-80019



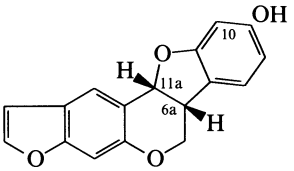
$C_{21}H_{26}O_7$ M 390.432
A disecopregnane derivative.

3-O-[α-L-Cymaropyranosyl-(1→4)-β-D-digitoxopyranosyl-(1→4)-β-D-oleandropyranoside]: ***Neocynaponoside A***
$C_{41}H_{60}O_{16}$ M 808.915
Constit. of *Cynanchum paniculatum*. Amorph. powder. Mp 105-108°. $[\alpha]_D$ −57.3° (c, 1.54 in $CHCl_3$).

Sugama, K. *et al*, *Phytochemistry*, 1988, **27**, 3984.

Neodunol N-80020

Updated Entry replacing N-50092
6a,11a-Dihydro-6H-benzofuro[3,2-c]furo[3,2-g][1]benzopyran-9-ol, 9CI
[53766-53-3]



$C_{17}H_{12}O_4$ M 280.279
Pterocarpan numbering shown. Isol. from *Neorautanenia edulis*, also from *N. amboensis* and *Pachyrrhizus erosus*. Cryst. (C_6H_6/hexane). Mp 170.5-171.5°. $[\alpha]_D^{22}$ −284.9° (c, 0.8 in $CHCl_3$).

Me ether: [53833-80-0].
$C_{18}H_{14}O_4$ M 294.306
Isol. from *Echinopora lamellosa*. Mp 175°. $[\alpha]_D^{25}$ −217° (c, 0.415 in $CHCl_3$).

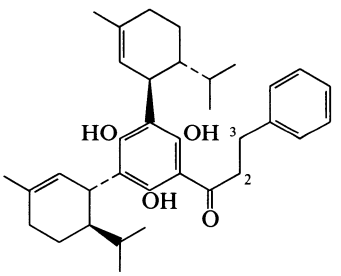
Me ether, 10-methoxy: [76165-15-6]. ***Ambonane***
$C_{19}H_{16}O_5$ M 324.332
Isol. from *N. amboenis* root bark. Light-yellow needles (Et_2O/hexane). Mp 125-127°. $[\alpha]_D$ −214° (c, 0.01 in $CHCl_3$).

6a,11a-Didehydro: [53766-54-4]. ***Neorauteen.*** *6H-Benzofuro[3,2-c]furo[3,2-g][1]benzopyran-9-ol, 9CI*
$C_{17}H_{10}O_4$ M 278.264
Isol. from *N. edulis* root bark. Plates (MeOH). Mp 202.5-204°.

6a,11a-Didehydro, Ac: Needles. Mp 197.5-199°.

Brink, A.J. *et al*, *Phytochemistry*, 1972, **16**, 273 (*isol*)
Brink, A.J. *et al*, *Phytochemistry*, 1974, **13**, 1581 (*Neorauteen*)
Ingham, J.L., *Z. Naturforsch.*, *C*, 1979, **34**, 683 (*isol*)
Breytenbach, J.C. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1980, 1804 (*Ambonane*)
Sanduja, R. *et al*, *J. Heterocycl. Chem.*, 1984, **21**, 845 (*isol, deriv, cryst struct, abs config*)

Neolinderatin N-80021



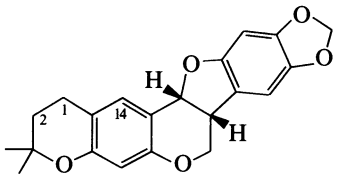
$C_{35}H_{46}O_4$ M 530.746
Constit. of *Lindera umbellata*. Viscous oil. $[\alpha]_D$ +20.3° (c, 0.9 in $CHCl_3$).

2,3-Didehydro: [120217-40-5]. ***Neolinderachalcone***
$C_{35}H_{44}O_4$ M 528.730
Constit. of *L. umbellata*. Viscous oil. $[\alpha]_D$ +26.5° (c, 0.15 in $CHCl_3$).

Ichino, K. *et al*, *Chem. Lett.*, 1989, 363 (*struct, synth*)

Neorautane N-80022

Updated Entry replacing N-10030
[36284-97-6]



Absolute configuration

$C_{21}H_{20}O_5$ M 352.386
CA numbering shown. Constit. of root bark of *Neorautanenia edulis*. Cryst. (MeOH). Mp 204°. $[\alpha]_D^{23}$ −255° (c, 1.4 in $CHCl_3$).

14-Methoxy: [63343-93-1]. ***Neorautanin***
$C_{22}H_{22}O_6$ M 382.412
From *N. edulis*. Needles (C_6H_6/hexane). Mp 202-204°. $[\alpha]_D^{21}$ −303° (c, 0.2 in $CHCl_3$).

1,2-Didehydro: [65418-33-9]. ***Neorautenane.*** *Neorautenaan*
$C_{21}H_{18}O_5$ M 350.370
Isol. from root bark of *N. amboensis*. Needles (EtOH). Mp 165-166°. $[\alpha]_D$ −200° (c, 0.1 in $CHCl_3$).

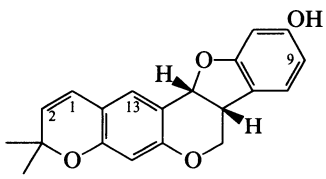
1,2-Didehydro, 14-hydroxy: [76175-39-8]. ***Neorautenanol***
$C_{21}H_{18}O_6$ M 366.370
Isol. from *N. amboensis*. Glass.

2ξ-Hydroxy: [76165-13-4]. ***Neorautanol***
$C_{21}H_{20}O_6$ M 368.385
Isol. from *N. amboensis* root bark. Glass. Mp 93-95°.

Rall, G.J. *et al*, *J. S. Afr. Chem. Inst.*, 1972, **25**, 25 (*isol*)
Brink, A.J. *et al*, *Phytochemistry*, 1977, **16**, 273 (*Neorautanin*)
Breytenbach, J.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1804 (*Neorautenane, Neorautanol, Neorautenanol*)

Neorautenol N-80023

Updated Entry replacing N-10031
[53766-52-2]



$C_{20}H_{18}O_4$ M 322.360
Isol. from *Neorautanenia edulis*. Cryst. (MeOH). Mp 168.5-170°. $[\alpha]_D^{22}$ −188.2° (c, 1.5 in $CHCl_3$).

13-Methoxy: [76165-14-5]. ***Edulenanol***
$C_{21}H_{20}O_5$ M 352.386
Constit. of *N. amboensis* root bark. Yellow glass. $[\alpha]_D$ −224° (c, 0.8 in $CHCl_3$).

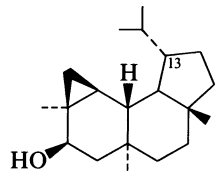
13-Methoxy, Me ether: [53734-77-3]. ***Edulenane.*** *Edulaan*
$C_{22}H_{22}O_5$ M 366.413
Constit. of *N. amboensis* root bark. Cubes (EtOH or Me_2CO), needles (EtOH). Mp 185-186°.

9,13-Dimethoxy: [56257-27-3]. ***Desmodin***
$C_{22}H_{22}O_6$ M 382.412
Isol. from *Desmodium gangeticum* roots. Cryst. Mp 236-238°.

13-Methoxy, Me ether, 1,2-dihydro: [37706-59-5]. ***Edulane***
$C_{22}H_{24}O_5$ M 368.429
Constit. of *N. edulis* root bark. Needles (C_6H_6). Mp 174-175°. $[\alpha]_D^{20}$ −258° (c, 0.2 in $CHCl_3$).

Brink, A.J. *et al*, *Phytochemistry*, 1974, **13**, 1581 (*isol, struct*)
Purushothaman, K.K. *et al*, *Phytochemistry*, 1975, **14**, 1129 (*Desmodin*)
Brink, A.J. *et al*, *Phytochemistry*, 1977, **16**, 273 (*Edulane*)
Chalmers, A.A. *et al*, *Tetrahedron*, 1977, **33**, 1735 (*cmr*)
Breytenbach, J.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1804 (*Edulenane, Edulenanol*)

5-Neoverrucosanol N-80024



$C_{20}H_{34}O$ M 290.488

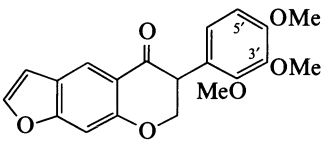
5β-form
Constit. of *Schistochila rigidula*.

13-Epimer: [116502-06-8]. ***13-Epi-5β-neoverrucosanol***
$C_{20}H_{34}O$ M 290.488
Constit. of *S. nobilis* and *Plagiochila stephensoniana*. Cryst. (hexane). Mp 151-153.5°. $[\alpha]_D$ +45.5° (c, 0.8 in $CHCl_3$).

Wu, C.-L. *et al*, *J. Hattori Bot. Lab.*, 1988, **64**, 151 (*isol*)
Fukuyama, Y. *et al*, *Phytochemistry*, 1988, **27**, 1797 (*isol, cryst struct*)
Asakawa, Y. *et al*, *Phytochemistry*, 1988, **27**, 3509 (*isol*)

Nepseudin N-80025

Updated Entry replacing N-00537
*6,7-Dihydro-6-(2,3,4-trimethoxyphenyl)-5*H*-furo[3,2-g][1]benzopyran-5-one, 9CI*
[20848-57-1]



$C_{20}H_{18}O_6$ M 354.359
Isol. from roots of *Neorautanenia pseudopachyrrhiza*. Cryst. ($CHCl_3$/MeOH). Mp 115-116°.

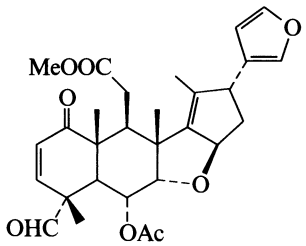
3′-Demethoxy: [76165-16-7]. ***Neoraunone***
$C_{19}H_{16}O_5$ M 324.332
Constit. of root bark of *N. amboensis*. Light-yellow needles (EtOH). Mp 154-155°. Opt. inactive.

3′-Demethoxy, 5′-methoxy: [76165-17-8]. ***Ambonone***
$C_{20}H_{18}O_6$ M 354.359
Constit. of root bark of *N. amboensis*. Light-yellow rosettes (C_6H_6). Mp 153-155°. Opt. inactive.

Fukui, K. *et al*, *Experientia*, 1963, **19**, 621 (*isol*)
Crombie, L. *et al*, *J. Chem. Soc.*, 1963, 1569 (*isol*)
Fukui, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 1385 (*synth*)
Breytenbach, J.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1804 (*Neoraunone, Ambonone*)

Nimbanal N-80026

[120462-51-3]

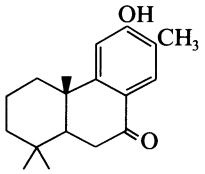


$C_{29}H_{34}O_8$ M 510.583
Constit. of *Azadirachta indica*. Cryst. (Me_2CO/pet. ether). Mp 195-197°. $[\alpha]_D$ +46° ($CHCl_3$).

Rajatkar, S.R. *et al*, *Phytochemistry*, 1989, **28**, 203.

Nimbiol N-80027

Updated Entry replacing N-00629
12-Hydroxy-13-methyl-8,11,13-podocarpatrien-7-one
[561-95-5]



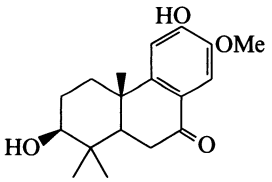
$C_{18}H_{24}O_2$ M 272.386
Constit. of *Melia azadirachta*. Cryst. Mp 244°. $[\alpha]_D$ +32.3° ($CHCl_3$).

Me ether: [123123-15-9]. ***Methylnimbiol***
$C_{19}H_{26}O_2$ M 286.413
Constit. of *Azadirachta indica*. Plates (hexane). Mp 142-143°.

Meyer, W.L. *et al*, *J. Org. Chem.*, 1975, **40**, 3686 (*isol*, *pmr*)
Ara, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1054 (*Methylnimbiol*)

Nimbionol N-80028

3β,12-Dihydroxy-13-methoxy-8,11,13-podocarpatrien-7-one

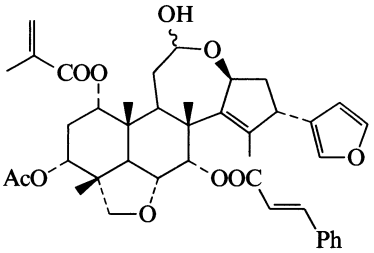


$C_{18}H_{24}O_4$ M 304.385
Constit. of *Azadirachta indica*. Needles ($CHCl_3$). Mp 127-129°. $[\alpha]_D$ +10° (c, 0.001 in $CHCl_3$).

3-Ketone: 12-Hydroxy-13-methoxy-8,11,13-podocarpatriene-3,7-dione. ***Nimbionone***
$C_{18}H_{22}O_4$ M 302.369
Constit. of *A. indica*. Plates ($CHCl_3$). Mp 78-79°. $[\alpha]_D$ +0.03° (c, 0.036 in $CHCl_3$).

Siddiqui, S. *et al*, *Phytochemistry*, 1988, **27**, 3903.

Nimbolicin N-80029

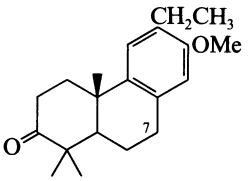


$C_{41}H_{48}O_{10}$ M 700.824
Constit. of *Azadirachta indica*. Plates. Mp 121-122°. $[\alpha]_D^{24}$ −33.3° ($CHCl_3$).

Ara, I. *et al*, *Heterocycles*, 1989, **29**, 729.

Nimbonolone N-80030

12-Ethyl-13-methoxy-8,11,13-podocarpatrien-3-one



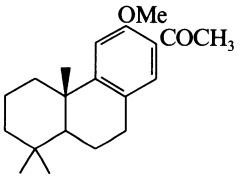
$C_{20}H_{28}O_2$ M 300.440
Constit. of *Azadirachta indica*. Cryst. (hexane). Mp 73-74°.

3-Deoxo, 7-oxo: 12-Ethyl-13-methoxy-8,11,13-podocarpatrien-7-one. ***Nimbonone***
$C_{20}H_{28}O_2$ M 300.440
Constit. of *A. indica*. Cryst. (hexane). Mp 68-69°. $[\alpha]_D$ +15° (c, 0.06 in $CHCl_3$).

Ara, I. *et al*, *Phytochemistry*, 1989, **28**, 1177.

Nimbosone N-80031

12-Methoxy-17-nor-8,11,13-abietatrien-15-one. 13-Acetyl-12-methoxy-8,11,13-podocarpatriene
[19889-21-5]

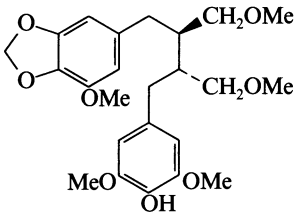


$C_{20}H_{28}O_2$ M 300.440
Constit. of *Azadirachta indica*. Needles (hexane). Mp 137-139°.

Ohashi, M. *et al*, *Tetrahedron Lett.*, 1968, 719 (*synth*)
Ara, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1054 (*isol*, *pmr*)

Nirphyllin N-80032

[120396-54-5]



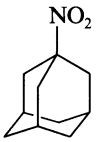
$C_{24}H_{32}O_8$ M 448.512
Constit. of *Phyllanthus niruri*.

Singh, B. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 48 (*isol, ir, pmr*)

1-Nitroadamantane N-80033

1-Nitrotricyclo[3.3.1.1^{3,7}]decane, 9CI

[7575-82-8]



$C_{10}H_{15}NO_2$ M 181.234
Waxy solid by subl. Mp 173° (158.5-159.0°).

Stetter, H. *et al*, *Chem. Ber.*, 1960, **93**, 226 (*synth*)
Smith, G.W. *et al*, *J. Org. Chem.*, 1961, **26**, 2207 (*synth, ir*)

2-Nitroadamantane N-80034

2-Nitrotricyclo[3.3.1.1^{3,7}]decane, 9CI

[54564-31-7]

$C_{10}H_{15}NO_2$ M 181.234
Cryst. (EtOH aq.). Mp 165-166°.

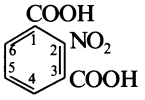
Bowan, W.R. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1980, 731 (*cmr*)
Archibald, T.G. *et al*, *J. Org. Chem.*, 1988, **53**, 4645 (*synth, ir, pmr*)

2-Nitro-1,3-benzenedicarboxylic acid, 9CI N-80035

Updated Entry replacing N-00712

2-Nitroisophthalic acid, 8CI

[21161-11-5]



$C_8H_5NO_6$ M 211.131
Prisms (MeOH). Mp 315°.

Mono-Me ester:
$C_9H_7NO_6$ M 225.157
Needles (H_2O). Mp 197°.

Di-Me ester: [57052-99-0].
$C_{10}H_9NO_6$ M 239.184
Needles (H_2O). Mp 135°.

Monoamide:
$C_8H_6N_2O_5$ M 210.146
Plates (MeOH). Mp 252°.

Diamide:
$C_8H_7N_3O_4$ M 209.161
Cryst. (H_2O). Mp 278-280°.

Dichloride:
$C_8H_3Cl_2NO_4$ M 248.021
Cryst. Mp 128-130°.

Nölting, E. *et al*, *Ber.*, 1906, **39**, 73 (*synth*)
Wohl, A., *Ber.*, 1910, **43**, 3474 (*synth, derivs*)
Isensee, R.W. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 4061.
Andrews, B.D. *et al*, *Aust. J. Chem.*, 1971, **24**, 413.
Harvey, I.W. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1939 (*synth, derivs*)

6-Nitro-4*H*-1-benzopyran-4-one N-80036

6-Nitrochromone

[51484-05-0]

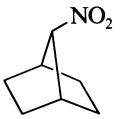
$C_9H_5NO_4$ M 191.143
Yellow solid (C_6H_6). Mp 173-175° (170-171°).

Ellis, G.P. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 2781 (*synth, pmr*)

7-Nitrobicyclo[2.2.1]heptane N-80037

7-Nitronorbornane

[100859-83-4]

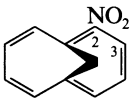


$C_7H_{11}NO_2$ M 141.169
Low-melting solid. Bp_7 170° (oven) .

Fukunaga, K. *et al*, *Synthesis*, 1987, 1097 (*synth, ir, pmr, ms*)

2-Nitrobicyclo[4.4.1]undeca-1,3,5,7,9-pentaene N-80038

2-Nitro-1,6-methano[10]annulene



$C_{11}H_9NO_2$ M 187.198
(±)-***form*** [118372-00-2]
Yellow oil.

Neidlein, R. *et al*, *Chem. Ber.*, 1989, **122**, 493 (*synth, pmr*)

3-Nitrobicyclo[4.4.1]undeca-1,3,5,7,9-pentaene N-80039

3-Nitro-1,6-methano-10-annulene

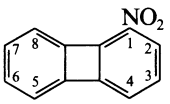
[118372-01-3]

$C_{11}H_9NO_2$ M 187.198

Neidlein, R. *et al*, *Chem. Ber.*, 1989, **122**, 493 (*synth, pmr*)

1-Nitrobiphenylene N-80040

[16294-08-9]



$C_{12}H_7NO_2$ M 197.193
Yellow needles (pet. ether). Mp 87-88°.

2,4,7-Trinitrofluorenone complex: [16294-07-8].
Red-brown plates (AcOH/EtOH). Mp 173-174°.

Barton, J.W. *et al*, *J. Chem. Soc. C*, 1967, 2097 (*synth, pmr*)

2-Nitrobiphenylene N-80041

[18931-53-8]

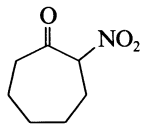
$C_{12}H_7NO_2$ M 197.193

Yellow needles (pet. ether). Mp 107-108°.

Baker, W. *et al*, *J. Chem. Soc.*, 1958, 2658, 2666 (*synth, uv*)

2-Nitrocycloheptanone N-80042

[13154-27-3]



$C_7H_{11}NO_3$ M 157.169

(±)-*form*

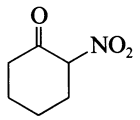
Cryst. (2-propanol). Mp 37.5-38.0°.

2,4-Dinitrophenylhydrazone: Mp 173-174°.

Feuer, H. *et al*, *J. Org. Chem.*, 1966, **31**, 3152 (*synth, ir*)

2-Nitrocyclohexanone N-80043

[4883-67-4]



$C_6H_9NO_3$ M 143.142

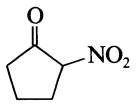
(±)-*form*

Cryst. solid. Mp 38°.

Wieland, W. *et al*, *Justus Liebigs Ann. Chem.*, 1928, **461**, 295 (*synth*)
Feuer, H. *et al*, *J. Org. Chem.*, 1966, **31**, 3152 (*synth, ir, pmr*)
Griswold, A.A. *et al*, *J. Org. Chem.*, 1966, **31**, 357 (*synth, ir*)
Dampawan, P. *et al*, *Synthesis*, 1983, 545 (*synth, ir*)

2-Nitrocyclopentanone N-80044

[22498-31-3]



$C_5H_7NO_3$ M 129.115

(±)-*form*

Yellow solid. Darkens on standing at r.t.

Elfehail, F. *et al*, *Synth. Commun.*, 1980, **10**, 929 (*synth, ir, pmr, uv*)

N-Nitrodimethylamine, 8CI N-80045

Updated Entry replacing N-00898

N-*Methyl*-N-*nitromethanamine*, *9CI*. *Dimethylnitramine*

[4164-28-7]

Me_2NNO_2

$C_2H_6N_2O_2$ M 90.082

Needles (ligroin). Sol. H_2O. Mp 58°. Bp 187°. Steam-volatile.

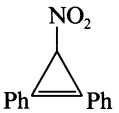
▷ Explosive >150°. Synth. produces carcinogenic byproducts. Causes exp. neoplasms. IQ0450000.

Robson, J.H. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 107 (*synth*)
Norris, W.P., *J. Am. Chem. Soc.*, 1959, **81**, 3346 (*synth*)
Boehme, H. *et al*, *Justus Liebigs Ann. Chem.*, 1965, **688**, 78 (*synth*)
Krebs, B. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 402 (*cryst struct*)
Bottaro, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 4140 (*synth, haz*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 859.

3-Nitro-1,2-diphenylcyclopropene N-80046

1,1'-(3-Nitro-1-cyclopropene-1,2-diyl)bisbenzene, *9CI*

[4949-78-4]



$C_{15}H_{11}NO_2$ M 237.257

Cryst. ($CHCl_3$/pet. ether). Mp 119° dec.

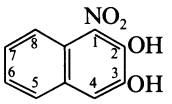
▷ Hazardous synth.

Jones, W.M. *et al*, *J. Org. Chem.*, 1965, **30**, 4389 (*synth, ir*)
Cheer, C.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 226 (*cryst struct, haz*)

1-Nitro-2,3-naphthalenediol, 9CI N-80047

Updated Entry replacing N-01050

2,3-Dihydroxy-1-nitronaphthalene



$C_{10}H_7NO_4$ M 205.170

Cryst. (EtOH aq.). Mp 210°.

Di-Me ether: [7311-21-9]. *2,3-Dimethoxy-1-nitronaphthalene*
$C_{12}H_{11}NO_4$ M 233.223
Pale yellow plates (EtOH). Mp 88.5-89°.

Bell, F., *J. Chem. Soc.*, 1959, 519 (*synth*)
Chang, C.W.J. *et al*, *J. Chem. Soc. C*, 1967, 840 (*deriv, pmr*)

1-Nitro-2,6-naphthalenediol, 9CI N-80048

2,6-Dihydroxy-1-nitronaphthalene

[104750-82-5]

$C_{10}H_7NO_4$ M 205.170

Mp 173°.

6-Me ether: [110387-94-5]. *6-Methoxy-1-nitro-2-naphthol*
$C_{11}H_9NO_4$ M 219.196
Mp >250°.

Di-Me ether: [39077-18-4]. *2,6-Dimethoxy-1-nitronaphthalene*
$C_{12}H_{11}NO_4$ M 233.223
Orange needles (C_6H_6). Mp 189°.

Chakravarti, S.N. *et al*, *J. Chem. Soc.*, 1937, 1859 (*synth, deriv*)
Mechin, B. *et al*, *Org. Magn. Reson.*, 1980, **14**, 79 (*cmr*)
Roussel, J. *et al*, *Tetrahedron Lett.*, 1986, **27**, 27 (*synth*)
Lemaire, M. *et al*, *Tetrahedron*, 1987, **43**, 835 (*synth, ir, pmr, deriv*)

1-Nitro-2,7-naphthalenediol, 9CI N-80049

Updated Entry replacing N-01051

2,7-Dihydroxy-1-nitronaphthalene

$C_{10}H_7NO_4$ M 205.170

Mp 198°.

Di-Me ether: [4614-14-6]. *2,7-Dimethoxy-1-nitronaphthalene*
$C_{12}H_{11}NO_4$ M 233.223
Yellow prisms (EtOH). Mp 141°.

Janczewski, M. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1961, **35**, 953 (*synth*)

Richer, J.C. *et al*, *Can. J. Chem.*, 1965, **43**, 3443 (*deriv, pmr*)
Mechin, B. *et al*, *Org. Magn. Reson.*, 1980, **14**, 79 (*cmr*)
Roussel, J. *et al*, *Tetrahedron Lett.*, 1986, **27**, 27 (*synth*)

2-Nitro-1,4-naphthalenediol, 9CI **N-80050**
1,4-Dihydroxy-2-nitronaphthalene
$C_{10}H_7NO_4$ M 205.170
Di-Me ether: [50885-07-9]. *1,4-Dimethoxy-2-nitronaphthalene*
$C_{12}H_{11}NO_4$ M 233.223
Cryst. Mp 97-98°.
Inoue, A. *et al*, *CA*, 1961, **55**, 13853e (*synth*)
Malesani, G. *et al*, *J. Heterocycl. Chem.*, 1985, **22**, 1141 (*pmr*)

2-Nitro-1,5-naphthalenediol **N-80051**
1,5-Dihydroxy-2-nitronaphthalene
[104750-78-9]
$C_{10}H_7NO_4$ M 205.170
Mp 226°.
Lemaire, M. *et al*, *Tetrahedron*, 1987, **43**, 835 (*synth, ir, pmr*)

2-Nitro-1,7-naphthalenediol **N-80052**
1,7-Dihydroxy-2-nitronaphthalene
[104750-80-3]
$C_{10}H_7NO_4$ M 205.170
Mp 220°.
Lemaire, M. *et al*, *Tetrahedron*, 1987, **43**, 835 (*synth, pmr, ir*)

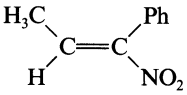
4-Nitro-1,2-naphthalenediol, 9CI **N-80053**
1,2-Dihydroxy-4-nitronaphthalene
$C_{10}H_7NO_4$ M 205.170
Di-Me ether: [42589-91-3]. *1,2-Dimethoxy-4-nitronaphthalene*
$C_{12}H_{11}NO_4$ M 233.223
Cryst. (EtOH). Mp 93-95.5°.
Archer, S. *et al*, *J. Med. Chem.*, 1980, **23**, 516 (*synth*)

4-Nitro-1,5-naphthalenediol, 9CI **N-80054**
1,5-Dihydroxy-4-nitronaphthalene
$C_{10}H_7NO_4$ M 205.170
Mp 187°.
5-Me ether: [110387-91-2]. *5-Methoxy-4-nitro-1-naphthol*
$C_{11}H_9NO_4$ M 219.196
Mp 165°.
Di-Me ether: 1,5-Dimethoxy-4-nitronaphthalene
$C_{12}H_{11}NO_4$ M 233.223
Yellow plates (AcOH). Mp 167°.
Thomson, R.H. *et al*, *J. Chem. Soc.*, 1947, 350 (*synth, deriv*)
Roussel, J. *et al*, *Tetrahedron Lett.*, 1986, **27**, 27 (*synth*)
Lemaire, M. *et al*, *Tetrahedron*, 1987, **43**, 835 (*synth, ir, pmr, deriv*)

4-Nitro-1,7-naphthalenediol, 9CI **N-80055**
4,6-Dihydroxy-1-nitronaphthalene
$C_{10}H_7NO_4$ M 205.170
Mp 240°.
Di-Me ether: [1143-67-5]. *4,6-Dimethoxy-1-nitronaphthalene*
$C_{12}H_{11}NO_4$ M 233.223
Cryst. (MeOH). Mp 127-128°.
Roussel, J. *et al*, *Tetrahedron Lett.*, 1986, **27**, 27 (*synth*)
Richer, J.C. *et al*, *Can. J. Chem.*, 1965, **43**, 715 (*synth, deriv, pmr*)
Mechin, B. *et al*, *Org. Magn. Reson.*, 1980, **14**, 79 (*cmr*)
Ferlin, M.G. *et al*, *J. Heterocycl. Chem.*, 1989, **26**, 245 (*synth, deriv*)

6-Nitro-2,3-naphthalenediol, 9CI **N-80056**
2,3-Dihydroxy-6-nitronaphthalene
$C_{10}H_7NO_4$ M 205.170
Di-Me ether: [14597-04-7]. *2,3-Dimethoxy-6-nitronaphthalene*
$C_{12}H_{11}NO_4$ M 233.223
Bright yellow needles (CCl_4). Mp 162-163°.
Chang, C.W.J. *et al*, *J. Chem. Soc. C*, 1967, 840 (*synth, deriv, pmr*)

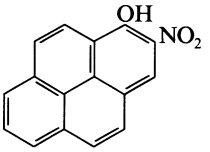
1-Nitro-1-phenylpropene **N-80057**
(1-Nitro-1-propenyl)benzene, 9CI
[25236-39-9]



(E)-form

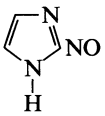
$C_9H_9NO_2$ M 163.176
$Bp_{0.5}$ 115°.
(E)-form [114390-79-3]
Yellow oil. Cont. 10% *Z*-isomer.
[114390-80-6]
Severin, T. *et al*, *Chem. Ber.*, 1969, **102**, 2966 (*synth*)
Asaro, F. *et al*, *Tetrahedron*, 1987, **43**, 3279 (*synth, ir, pmr, cmr*)

2-Nitro-1-pyrenol, 9CI **N-80058**
1-Hydroxy-2-nitropyrene
[113093-71-3]



$C_{16}H_9NO_3$ M 263.252
1983 and 1984 refs. descr. this compound as 1-nitro-2-pyrenol. Deep red needles (C_6H_6). Mp 227-229°.
▷ Potent mutagen.
Yashura, A. *et al*, *Chem. Lett.*, 1983, 347 (*synth, ir, pmr, ms*)
Löfroth, G. *et al*, *Z. Naturforsch., C*, 1984, **39**, 193.
Van den Braken-van Leersum, A.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1156 (*synth, pmr, ms, struct*)

2-Nitrosoimidazole **N-80059**

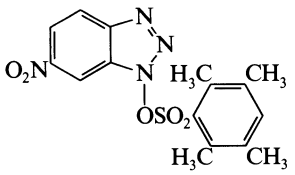


$C_3H_3N_3O$ M 97.076
N-*Me:* [116169-87-0]. *1-Methyl-2-nitroso-1H-imidazole*
$C_4H_5N_3O$ M 111.103
Green solid.
▷ Highly cytotoxic.
Noss, M.B. *et al*, *Biochem. Pharmacol.*, 1988, **37**, 2585 (*synth*)
Bolton, J.L. *et al*, *Can. J. Chem.*, 1988, **66**, 3044 (*struct, pmr*)

6-Nitro-1-[[(2,3,5,6-tetramethylphenyl) sulfonyl]oxy]-1*H*-benzotriazole, 9CI **N-80060**

1-(3-Durenesulfonyloxy)-6-nitrobenzotriazole

[117678-83-8]



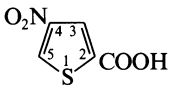
$C_{16}H_{16}N_4O_5S$ M 376.392

Improved reagent for ribonucleotide synth. by the triester method. Yellow cryst. (cyclohexane/toluene). Mp 158°.

Losse, G. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 19 (*synth, use*)

4-Nitro-2-thiophenecarboxylic acid, 9CI **N-80061**

[13138-70-0]



$C_5H_3NO_4S$ M 173.149

Glistening platelets (C_6H_6). Mp 154°.

Me ester: [24647-78-7].

$C_6H_5NO_4S$ M 187.176

Cryst. (Et_2O). Mp 98-100°.

Rinkes, I.J., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1932, **51**, 1134; 1933, **52**, 538 (*synth*)

Gever, G., *J. Am. Chem. Soc.*, 1953, **75**, 4585 (*synth, deriv*)

Noto, R. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1987, 689 (*cmr*)

Elliott, R. *et al*, *Tetrahedron*, 1987, **43**, 3295 (*synth, ir, pmr*)

5-Nitro-2-thiophenecarboxylic acid **N-80062**

[6317-37-9]

$C_5H_3NO_4S$ M 173.149

Needles (H_2O). Mp 158°.

Me ester: [5832-01-9].

$C_6H_5NO_4S$ M 187.176

Needles (pet. ether). Mp 76°.

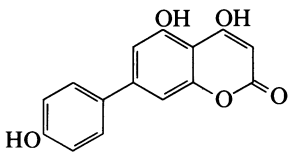
Rinkes, I.J., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1932, **51**, 1134; 1933, **52**, 538 (*synth*)

Noto, R. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1987, 689 (*cmr*)

Nivegin **N-80063**

*4,5-Dihydroxy-7-(4-hydroxyphenyl)-2*H*-1-benzopyran-2-one*

[114020-35-8]



$C_{15}H_{10}O_5$ M 270.241

Constit. of *Echinops niveus*. Cryst. Mp 262-264°.

Parmar, V.S. *et al*, *Tetrahedron*, 1989, **45**, 1839.

15-Nonacosanol, 9CI **N-80064**

[2764-81-0]

$$H_3C(CH_2)_{13}CH(OH)(CH_2)_{13}CH_3$$

$C_{29}H_{60}O$ M 424.792

Isol. from wax of *Arbutus unedo* and Brussels sprouts. Mp 83.1-83.8°.

Sahai, P.N. *et al*, *Biochem. J.*, 1932, **26**, 403 (*isol*)

Soza, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1950, **230**, 995 (*isol*)

1-Nonacosanol **N-80065**

[6624-76-6]

$$H_3C(CH_2)_{27}CH_2OH$$

$C_{29}H_{60}O$ M 424.792

Isol. from leaf wax of *Agave sisalana*. Cryst. (C_6H_6). Mp 85°.

Piper, S.H. *et al*, *Biochem. J.*, 1934, **28**, 2175 (*synth*)

Razafindrazaka, J. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1633 (*isol*)

Rao, S.J. *et al*, *Indian J. Chem., Sect. B*, 1987, **26**, 208 (*synth*)

15-Nonacosanone, 9CI **N-80066**

Ditetradecyl ketone. Dimyristyl ketone

[2764-73-0]

$$H_3C(CH_2)_{13}CO(CH_2)_{13}CH_3$$

$C_{29}H_{58}O$ M 422.777

Isol. from cabbage leaves (*Brassica oleracea*). Platelets (C_6H_6/EtOH). Mp 80.5-81°.

Collison, D.L. *et al*, *Biochem. J.*, 1931, **25**, 606 (*isol*)

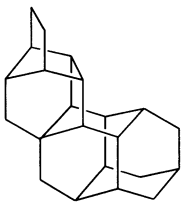
Kolattukudy, P.E., *Biochemistry*, 1965, **4**, 1844 (*biosynth*)

Matsota, N.P. *et al*, *Zh. Prikl. Khim.* (*Leningrad*), 1971, **44**, 1823; *ca*, **76**, 3358c (*synth*)

Nonacyclo[11.7.1.1^{2,18}.0^{3,16}.0^{4,13}.0^{5,10}.0^{6,14}.0^{7,11}.0^{15,20}]docosane **N-80067**

*Hexadecahydro-10*a*,1,4-ethanylylidene-7,5,9,11-[1,2]propanediyl[3]ylidene-10*aH*-benzo[b]fluorene, 9CI. Bastardane*

[20497-81-8]



$C_{22}H_{28}$ M 292.463

Cryst. (Me_2CO/hexane or by subl.). Mp 144.5-146.5°.

von Schleyer, P.R. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5034 (*synth, pmr, cryst struct*)

Osawa, E. *et al*, *J. Org. Chem.*, 1980, **45**, 2985 (*synth*)

6,8-Nonadien-1-ol **N-80068**

[74206-16-9]

$$H_2C{=}CHCH{=}CH(CH_2)_4CH_2OH$$

$C_9H_{16}O$ M 140.225

(E)-form

Oil.

Yasuda, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 1089 (*synth, ir, pmr*)

Vedejs, E. *et al*, *J. Org. Chem.*, 1988, **53**, 2220 (*synth, ir, pmr*)

1,3-Nonadiyne N-80069

[77657-83-1]

$H_3C(CH_2)_4C{\equiv}CC{\equiv}CH$

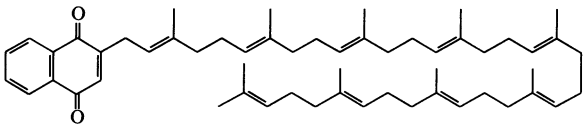
C_9H_{12} M 120.194

Kende, A.S. *et al*, *J. Org. Chem.*, 1988, **53**, 2655 (*synth, ir, pmr, ms*)

2-(3,7,11,15,19,23,27,31,35-Nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonenyl)-1,4-benzoquinone, 9CI N-80070

2-Solanesyl-1,4-naphthoquinone. Desmethylmenaquinone-9

[2197-56-0]



$C_{55}H_{78}O_2$ M 771.220

Prod. by *Streptococcus faecalis*. Yellow.

[20741-09-7]

Baum, R.H. *et al*, *J. Biol. Chem.*, 1963, **238**, PC4109; 1965, **240**, 3425 (*isol, uv, pmr, struct*)

2,3,5-Nonatriene N-80071

[115942-23-9]

$H_3CCH_2CH_2CH{=}CHCH{=}C{=}CHCH_3$

C_9H_{14} M 122.210

Reich, H.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6432 (*synth, pmr, ir, cmr*)

4-Nonene-6,8-diyn-1-ol, 9CI N-80072

$HC{\equiv}CC{\equiv}CCH{=}CHCH_2CH_2CH_2OH$

$C_9H_{10}O$ M 134.177

(E)-form

Isol. from *Aleurodiscus roseus*. Amorph. λ_{max} 229, 238, 251, 265, 281 nm. Not obt. completely pure.

Cambie, R.C. *et al*, *J. Chem. Soc.*, 1963, 4120 (*isol, uv, ir*)

3-Nonen-1-yne N-80073

$H_3C(CH_2)_4CH{=}CHC{\equiv}CH$

C_9H_{14} M 122.210

(E)-form

Liq. Bp_{90} 91.5-92°.

Andreini, B.P. *et al*, *Tetrahedron*, 1987, **43**, 4591 (*synth, pmr*)

2-Nonyn-1-ol, 9CI N-80074

Updated Entry replacing N-01595

[5921-73-3]

$H_3C(CH_2)_5C{\equiv}CCH_2OH$

$C_9H_{16}O$ M 140.225

Liq. with weak odour. Fp −21° (−16°). Bp_{17} 114-116°, Bp_{11} 109°.

3,5-Dinitrobenzoyl: Cryst. (ligroin). Mp 50°.

Me ether: [34498-02-7]. *1-Methoxy-2-nonyne, 9CI*

$C_{10}H_{18}O$ M 154.252

Oil.

Conia, J.M., *Bull. Soc. Chim. Fr.*, 1955, 1449 (*synth*)

Jones, V.K. *et al*, *J. Org. Chem.*, 1965, **30**, 3978 (*synth, spectra*)

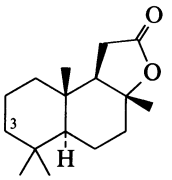
Ermilova, E.V. *et al*, *Zh. Org. Khim.*, 1975, **11**, 520 (*synth*)

Fortunato, J.M. *et al*, *J. Org. Chem.*, 1976, **41**, 2194 (*synth*)

Zhai, D. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2501 (*ether, synth, pmr, ir, ms*)

Norambreinolide N-80075

Updated Entry replacing N-40065



(+)-*form*

$C_{16}H_{26}O_2$ M 250.380

(+)-form [564-20-5]

Degradn. prod. of ambrein, etc. Found in tobacco. Cryst. (pet. ether or MeOH aq.). Mp 122-125°. $[\alpha]_D$ +42° (c, 0.25 in $CHCl_3$).

3α-Hydroxy: [123844-63-3]. ***3α-Hydroxynorambreinolide***

$C_{16}H_{26}O_3$ M 266.380

Constit. of *Salvia aethiopis*. Cryst. (Et_2O/hexane). Mp 190-191°. $[\alpha]_D$ +22.2° (c, 1.08 in $CHCl_3$).

(−)-form [95406-08-9]

ent-*Norambreinolide*

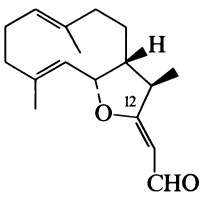
Constit. of *Sideritis nutans*. Cryst. (EtOAc/pet. ether). Mp 120-122°.

Carman, R.M., *Aust. J. Chem.*, 1966, **19**, 1535 (*synth, bibl*)

Fernández, C. *et al*, *Phytochemistry*, 1985, **24**, 188 (*isol*)

Gonzalez, M.S. *et al*, *Tetrahedron*, 1989, **45**, 3575 (*3α-Hydroxynorambreinolide*)

Norasperenal A N-80076



$C_{17}H_{24}O_2$ M 260.375

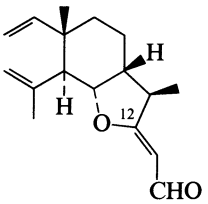
Metabolite of gorgonian *Eunicea* sp. Solid. Mp 101.5-102.5°. $[\alpha]_D$ +131° (c, 1.2 in MeOH).

12E-isomer: ***Norasperenal C***

Metabolite of *E.* species. Unstable oil.

Shin, J. *et al*, *Tetrahedron Lett.*, 1989, **30**, 6821.

Norasperenal B N-80077



$C_{17}H_{24}O_2$ M 260.375

Metabolite of gorgonian *Eunicea* sp. Solid. Mp 123-124.5°. $[\alpha]_D$ −23° (c, 0.5 in MeOH).

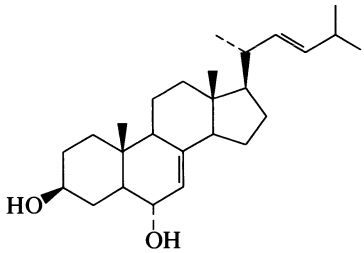
12E-Isomer: ***Norasperenal D***

$C_{17}H_{24}O_2$ M 260.375

Metab. of *E.* sp. Unstable oil.

Shin, J. *et al*, *Tetrahedron Lett.*, 1989, **30**, 6821.

24-Nor-7,22-cholestadiene-3,6-diol N-80078



$C_{26}H_{42}O_2$ M 386.617

(3β,5α,6α,22E)-form

Constit. of *Spongionella gracilis*. Cryst. (MeOH/pet. ether). Mp 188-190°.

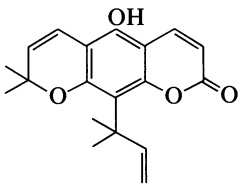
Madaio, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 952 (*isol*, *pmr*)

Nordentatin N-80079

Updated Entry replacing P-30169

10-(1,1-Dimethyl-2-propenyl)-5-hydroxy-8,8-dimethyl-2H,8H-benzo[1,2-b:5,4-b′]dipyran-2-one, *9CI*

[17820-07-4]



$C_{19}H_{20}O_4$ M 312.365

Constit. of roots of *Clausena dentata*. Mp 182°. Struct. revised in 1973.

Me ether: [22980-57-0]. ***Ponicitrin.*** *Dentatin*

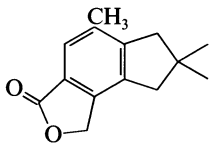
From *C. dentata* and from roots of *Poncirus trifoliata*. Pillars (EtOH). Mp 93-94°.

O(*1,1-Dimethyl-2-propenyl*): ***Ponfolin***

Isol. from roots of *P. trifoliata*. Oil.

Tomimatsu, T. *et al*, *Tetrahedron*, 1972, **28**, 2003 (*isol*, *uv*, *pmr*)
Mahey, S. *et al*, *Indian J. Chem.*, 1973, **11**, 983 (*synth*)
Mowat, D. *et al*, *Tetrahedron*, 1973, **29**, 2943 (*synth*)
Tomimatsu, T. *et al*, *Tetrahedron*, 1974, **30**, 939 (*struct*)
Murray, R.D.H. *et al*, *Tetrahedron Lett.*, 1983, **24**, 3773 (*synth*)
Furukawa, H. *et al*, *Chem. Pharm. Bull.*, 1986, **34**, 3922 (*Ponfolin*)

8-Norlactaranelactone N-80080

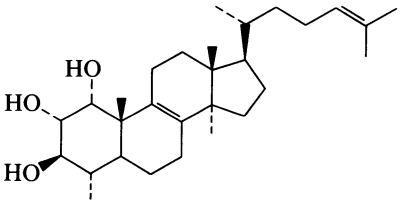


$C_{14}H_{16}O_2$ M 216.279

Constit. of *Lactarius serobiculatus*. Cryst. Mp 93-96°.

Bosetti, A. *et al*, *Phytochemistry*, 1989, **28**, 1427.

29-Nor-8,24-lanostadiene-1,2,3-triol N-80081



$C_{29}H_{48}O_3$ M 444.696

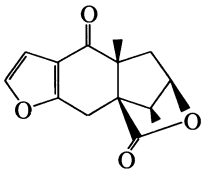
(1α,2α,3β)-form [119765-92-3]

Constit. of *Commiphora incisa*. Amorph. $[\alpha]_D$ +38.2° (c, 0.1 in $CHCl_3$).

Provan, G.J. *et al*, *Phytochemistry*, 1988, **27**, 3841.

Norpinguisanolide N-80082

[119285-62-0]



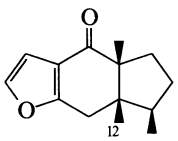
$C_{14}H_{14}O_4$ M 246.262

Constit. of *Porella elegantula*. Plates (hexane). Mp 132-134°. $[\alpha]_D^{22}$ −125° (c, 0.47 in $CHCl_3$).

Fukuyama, Y. *et al*, *Phytochemistry*, 1988, **27**, 3557 (*isol*, *pmr*)

Norpinguisone N-80083

[62121-27-1]



$C_{14}H_{18}O_2$ M 218.295

Constit. of *Porella vernicosa* and *P. elegantula*. Cryst. Mp 126-127°. $[\alpha]_D$ +2° ($CHCl_3$).

12-Carboxylic acid, Me ester: [119285-56-2]. *Methyl 4-oxonorpinguisan-12-oate. Norpinguisone methyl ester* (*incorr.*)

$C_{15}H_{18}O_4$ M 262.305

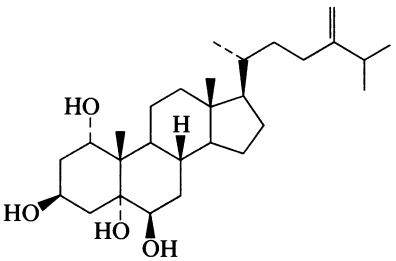
Constit. of *P. vernicosa* and *P. elegantula*. Oil. $[\alpha]_D^{16}$ −60.2° (c, 0.91 in $CHCl_3$).

[67594-77-8]

Asakawa, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1976, 1469 (*isol*)
Fukuyama, Y. *et al*, *Phytochemistry*, 1988, **27**, 3557 (*isol*, *struct*)

Numersterol A N-80084

24-Methylene-1α,3β,5α,6β-cholestanetetrol



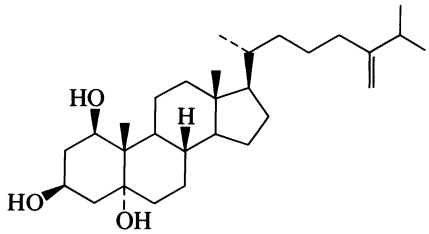
$C_{28}H_{48}O_4$ M 448.685

Constit. of *Sinularia numerosa*. Cryst. (MeOH). Mp 297-299°. $[\alpha]_D^{25}$ +4.5° (c, 0.332 in MeOH).

Su, J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 934 (*isol*, *pmr*, *cmr*, *cryst struct*)

Numersterol B N-80085

25-Methylene-22-homocholestane-1β,3β,5α-triol. 27,27-Dimethyl-25-cholestene-1β,3β,5α-triol



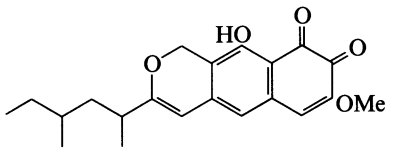
$C_{29}H_{50}O_3$ M 446.712

Constit. of *Sinularia numerosa*. Cryst. (Me_2CO/pet. ether). Mp 121-122°.

Su, J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 934 (*isol*, *pmr*, *cmr*)

O

Obionin A — O-80001

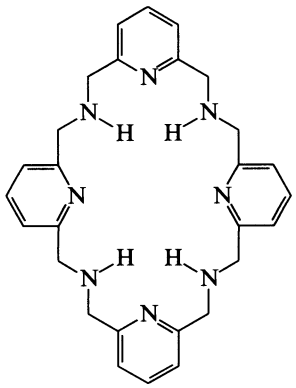


$C_{21}H_{24}O_5$ M 356.418
Metab. of marine fungus *Leptosphaeria obiones*. Brown-red solid. Mp 168-169°. $[\alpha]_D$ +28.5° (c, 0.01 in $CHCl_3$).

Poch, G.K. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3483.

3,11,19,27,33,34,35,36-Octaazapentacyclo [27.3.1.1^{5,9}.1^{13,17}.1^{21,25}]hexatriaconta-1(33),5(34),6,8,13,(35),14,16,21(36),22, 24,29,31-dodecaene — O-80002

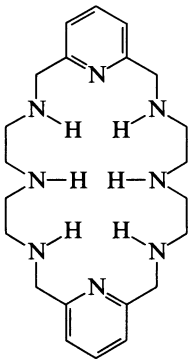
Cyclotetra(2,6-pyridinemethyleneimine)



$C_{28}H_{32}N_8$ M 480.614
B,5HCl: Mp >260°.
N-*Tetrakis(4-methylbezenesulfonyl):* Mp >260°.

Hosseini, M.W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1066 (*synth*)

3,6,9,17,20,23,29,30-Octaazatricyclo [23.3.1.1^{11,15}]triaconta-1(29),11(30),12, 14,25,27-hexaene — O-80003



$C_{22}H_{34}N_8$ M 410.564
B,8HCl: Tetrahydrate. Mp 228°.
N-*Hexakis-(4-methylbenzenesulfonyl):* Cryst. (CH_2Cl_2/hexane/DMF). Mp 142°.

Hosseini, M.W. *et al*, *Helv. Chim. Acta*, 1989, **72**, 1066 (*synth*)

Octachloropropane — O-80004

Perchloropropane
[594-90-1]

$Cl_3CCCl_2CCl_3$

C_3Cl_8 M 319.655
Oil. Bp 280°, Bp_{734} 268-269°.

Kraft, F. *et al*, *Ber.*, 1875, **8**, 1296 (*synth*)
Farah, B.S. *et al*, *J. Org. Chem.*, 1965, **30**, 1241 (*synth*)

Octacosanal — O-80005

[22725-64-0]

$H_3C(CH_2)_{26}CHO$

$C_{28}H_{56}O$ M 408.750
Isol. from wax of grapes (*Vitis vinifera*) and from cabbage leaves (*Brassica oleracea*).

Radler, F. *et al*, *Aust. J. Chem.*, 1965, **18**, 1059 (*isol*)
Schmid, H.H.O. *et al*, *Hoppe Seyler's Z. Physiol. Chem.*, 1969, **350**, 462 (*isol*)

11,17-Octadecadien-9-ynoic acid, 9CI — O-80006

$H_2C{=}CH(CH_2)_4CH{=}CHC{\equiv}C(CH_2)_7COOH$

$C_{18}H_{28}O_2$ M 276.418
(E)-form [5910-97-4]
Isol. from seed oil of *Acanthosyris spinescens* and *Pyrucaria pubera*. Cryst. (hexane). Mp 30.0-34.5°.
Me ester: [20714-98-1].
$C_{19}H_{30}O_2$ M 290.445
Liq.
4-Phenylphenacyl ester: [20714-99-2].
Cryst. (EtOH). Mp 53-54°.

Powell, R.G. *et al*, *Biochemistry*, 1966, **5**, 625 (*isol, uv, ir, pmr, struct*)
Hopkins, C.Y. *et al*, *J. Chem. Soc. C*, 1968, 2462 (*isol, uv, ir, pmr*)

2-Octadecanol, 9CI — O-80007

[593-32-8]

$H_3C(CH_2)_{15}CH(OH)CH_3$

$C_{18}H_{38}O$ M 270.498
(+)-form [23559-98-0]
Isol. from avian tubercle bacillus wax. Needles (MeOH). Mp 56°. $[\alpha]_D^{25}$ +5.7° ($CHCl_3$).
Phenylurethane: Long fine needles. Mp 76-77°. $[\alpha]_D^{22}$ +7.9° ($CHCl_3$).
3,5-Dinitrobenzoyl: Cryst. (EtOH). Mp 71-72°. $[\alpha]_D$ +25.3° ($CHCl_3$).

Pangborn, M.C. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 10 (*isol*)
Reeves, R.E. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 858 (*isol*)
Tulloch, A.P., *Can. J. Chem.*, 1968, **46**, 3727 (*synth, pmr*)

4,8,12,15-Octadecatetraenoic acid, 9CI O-80008

[67329-10-6]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2COOH$

$C_{18}H_{28}O_2$ M 276.418
Isol. from sardine oil, from seeds of *Lithospermum officinale* and from *Salpa thomsoni*.

[106440-10-2]

Toyama, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1935, **10**, 232 (*isol*)
Hörhammer, L. *et al*, *Arzneim.-Forsch.*, 1964, **14**, 34 (*isol*)
Mimura, T. *et al*, *Chem. Pharm. Bull.*, 1986, **34**, 4562 (*isol*)

15-Octadecene-9,11,13-triynoic acid O-80009

$H_3CCH_2CH{=}CH(C{\equiv}C)_3(CH_2)_7COOH$

$C_{18}H_{22}O_2$ M 270.371
Major component of the lipids of *Santalum acuminatum*.
λ_{max} 212, 223, 232, 244, 258, 274, 291, 310, 332 nm.

Bu'Lock, J.D. *et al*, *Phytochemistry*, 1963, **2**, 289.

17-Octadecen-9-ynoic acid O-80010

$H_2C{=}CH(CH_2)_6C{\equiv}C(CH_2)_7COOH$

$C_{18}H_{30}O_2$ M 278.434
Isol. from seed oil of *Acanthosyris spinescens*.

Powell, R.G. *et al*, *Biochemistry*, 1966, **5**, 625.

2,6-Octadienoic acid O-80011

$H_3CCH{=}CHCH_2CH_2CH{=}CHCOOH$

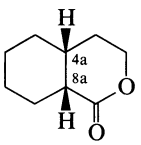
$C_8H_{12}O_2$ M 140.182

(E,E)-form [116565-36-7]
Waxy solid. Mp 44-46°.

Me ester: [25172-05-8].
$C_9H_{14}O_2$ M 154.208
Liq.

Crandall, J.K. *et al*, *J. Org. Chem.*, 1970, **35**, 3049 (*synth, ir, pmr*)
Snider, B.B., *J. Org. Chem.*, 1988, **53**, 5320 (*synth, pmr, cmr, ir*)

Octahydro-1*H*-2-benzopyran-1-one O-80012



(4*aRS*,8*aRS*)-*form*

$C_9H_{14}O_2$ M 154.208

(4aRS,8aRS)-form
(±)-cis-*form*
Liq. $Bp_{4.5}$ 118°.

Hydrazide: Needles (EtOH/Et_2O). Mp 109-110°.

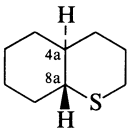
(4aRS,8aSR)-form
(±)-trans-*form*
Prisms. Mp 48°. Bp_3 103°.

Hydrazide: Prisms. Mp 123-124°.

Fujiwara, Y. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1458 (*synth*)

Octahydro-2*H*-1-benzothiopyran, 9CI O-80013

Updated Entry replacing O-20017
1-Thiadecalin
[29100-30-9]



(8*aR*,4*aS*)-*form*

$C_9H_{16}S$ M 156.291

(8aR,4aS)-form [116782-11-7]
(+)-trans-form
Solid. Mp 34.5-35.0°. Bp_1 110°. $[\alpha]_D^{26}$ +24.4° (c, 6.15 in MeOH).

1,1-Dioxide: [116782-13-9].
$C_9H_{16}O_2S$ M 188.290
Cryst. (hexane). Mp 103-103.2°. $[\alpha]_D^{29}$ +3.5° (c, 6.39 in MeOH).

(4aRS,8aRS)-form [57259-80-0]
(±)-cis-*form*
Mp −1° to 1°.

$HgCl_2$ complex: [63714-82-9].
Mp 176-177°.

(4aRS,8aSR)-form [54340-73-7]
(±)-trans-*form*. 4aα,8aβ-*form*
Mp 17-18°.

$HgCl_2$ complex: [63743-83-9].
Mp 170-171°.

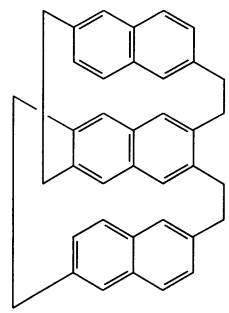
1α-Oxide: [67530-10-3].
$C_9H_{16}OS$ M 172.291
Mp 87-88°.

1β-Oxide: [67530-09-0].
$C_9H_{16}OS$ M 172.291
Mp 71-72°.

Claus, P.K. *et al*, *J. Org. Chem.*, 1977, **42**, 4016 (*synth*)
Oae, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 270 (*oxides*)
Cerè, V. *et al*, *J. Org. Chem.*, 1988, **53**, 5689 (*synth, cmr, pmr*)

5,6,15,16,19,20,29,30-Octahydro-2,17:3,18:7,11:10,14:21,25:24,28-hexamethenobenzocyclooctacosene, 9CI O-80014

[88903-18-8]



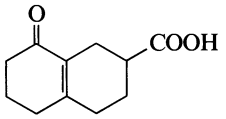
$C_{38}H_{32}$ M 488.671
Prisms. Mp 230° dec.

Otsubo, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1989, **62**, 164 (*synth, cryst struct*)

1,2,3,4,5,6,7,8-Octahydro-8-oxo-2-naphthalenecarboxylic acid, 9CI O-80015

$\Delta^{9,10}$-Octal-1-one-7-carboxylic acid. 3,4,5,6,7,8-Hexahydronaphthalen-1(2H)-one-2-carboxylic acid

[32178-64-6]



$C_{11}H_{14}O_3$ M 194.230

(±)-***form*** [112400-28-9]

Needles (MeCN aq.). Mp 145-147°.

Me ester:

$C_{12}H_{16}O_3$ M 208.257

Intermed. for terpene synth. $Bp_{0.11}$ 119-122°.

Me ester, 2,4-dinitrophenylhydrazone: Red cryst. (MeOH/EtOAc). Mp 194.5-196.5°.

Et ester: [112400-24-5].

$C_{13}H_{18}O_3$ M 222.283

Oil.

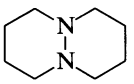
[34407-92-6]

Huffman, J.W. *et al*, *J. Org. Chem.*, 1972, **37**, 13 (*synth, ir, uv, pmr*)
Carlson, R.G. *et al*, *J. Org. Chem.*, 1972, **37**, 2468 (*synth, ir, uv, pmr*)
Strekowski, L. *et al*, *J. Org. Chem.*, 1988, **53**, 901 (*synth*)

Octahydropyridazino[1,2-*a*]pyridazine, 9CI O-80016

1,6-Diazabicyclo[3.3.0]decane. 4a,8a-Diazadecalin. 10-Azaquinolizidine

[3661-15-2]



$C_8H_{16}N_2$ M 140.228

Oil. Bp_5 40°. Forms a cryst. monohydrate.

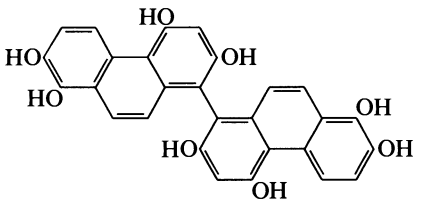
B,HClO$_4$: Mp 231°.

Picrate: Mp 155°.

Hedaya, E. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 3052 (*synth*)
Koopmann, H.P. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 157 (*ir, raman*)
Nelsen, S.F. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 4004 (*cmr*)
Nelsen, S.F. *et al*, *J. Org. Chem.*, 1980, **45**, 3609 (*nmr*)
White, J.M. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 1777 (*cryst struct*)

2,2′,4,4′,7,7′,8,8′-Octahydroxy-1,1′-biphenanthrene O-80017

[1,1′-Biphenanthrene]-2,2′,4,4′,7,7′,8,8′-octol



$C_{28}H_{18}O_8$ M 482.445

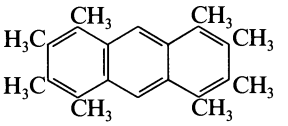
4,4′,8,8′-Tetra-Me ether: [118201-23-3]. *2,2′,7,7′-Tetrahydroxy-4,4′8,8′-tetramethoxy-1,1′-biphenanthrene. 4,4′,8,8′-Tetramethoxy-[1,1′-biphenanthrene]-2,2′,7,7′-tetrol*

$C_{32}H_{26}O_8$ M 538.553

Constit. of *Eulophia nuda*. Pink needles ($Et_2O/CHCl_3/Me_2CO$). Mp 310° dec.

Tuchinda, P. *et al*, *Phytochemistry*, 1988, **27**, 3267.

1,2,3,4,5,6,7,8-Octamethylanthracene O-80018



$C_{22}H_{26}$ M 290.447

Yellow cryst. powder (chlorobenzene). Mp 299-300°. Fluor. in soln.

Backer, H.J. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1939, **58**, 761 (*synth*)
Krysin, A.P. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1977, **13**, 1183 (*synth, uv, pmr*)
Hart, H. *et al*, *J. Org. Chem.*, 1981, **46**, 1251 (*synth*)
Meador, M.A. *et al*, *J. Org. Chem.*, 1989, **54**, 2336 (*synth, pmr*)

1,2,4-Octatriene O-80019

$H_3CCH_2CH_2CH{=}CHCH{=}C{=}CH_2$

C_8H_{12} M 108.183

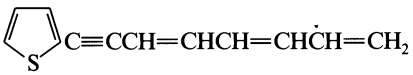
(*E*)-***form*** [115942-28-4]

Liq.

Reich, H.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6432 (*synth, pmr, ir, cmr*)

2-(3,5,7-Octatrien-1-ynyl)thiophene O-80020

8-(2-Thienyl)-1,3,5-octatriene-7-yne



$C_{12}H_{10}S$ M 186.277

Isol. from roots of *Matricaria invdora, M. oreades* and *Xeranthemum cylindraceum*. Cryst. or oil. Mp 48°. Prob. a mixt. of geom. isomers as isolated. Mp. refers to synthetic material (geom. isom. not reported).

Sörensen, N.A., *Proc. Chem. Soc., London*, 1961, 98 (*struct, synth*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 1193, 2125 (*isol, struct, uv, ir, pmr, synth*)

2-Octenedial O-80021

[105582-16-9]

$OHC(CH_2)_4CH{=}CHCHO$

$C_8H_{12}O_2$ M 140.182

[41980-05-6]

Carlson, R.G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 223 (*synth*)
Hudlicky, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4735 (*synth, ir, pmr*)

5-Octenoic acid O-80022

[63892-00-2]

$H_3CCH_2CH{=}CHCH_2CH_2CH_2COOH$

$C_8H_{14}O_2$ M 142.197

(*E*)-***form*** [16424-53-6]

$Bp_{1.5}$ 120°.

[41653-97-8]

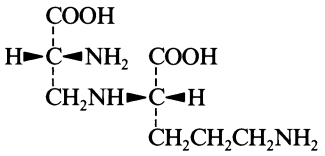
Scholz, D., *Justus Liebigs Ann. Chem.*, 1984, 264.
Kawashima, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255.

Octopinic acid O-80023

Updated Entry replacing O-00426

N^2-(*1-Carboxyethyl*)*ornithine*, *9CI*

[20197-09-5]



$C_8H_{16}N_2O_4$ M 204.225

Amino acid found in crown gall tissue of *Scorzonera* root infected with *Agrobacterium tumefaciens*. Mp 270-271° dec. $[\alpha]_D^{20}$ +18.5° (c, 0.5 in H_2O).

Lejeune, B., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. D*, 1967, **265**, 1753 (*synth*)

Goto, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 261 (*synth*)

7-Octynoic acid O-80024

[10297-09-3]

$HC{\equiv}C(CH_2)_5COOH$

$C_8H_{12}O_2$ M 140.182

Liq. $Bp_{0.4}$ 96-97°.

Anhydride: [119837-88-6].

$C_{16}H_{22}O_3$ M 262.348

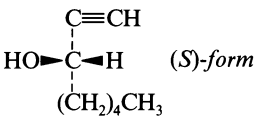
Liq. Bp_1 160-166°.

Moody, C.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3249 (*synth, anhydride, ir, pmr, ms*)

1-Octyn-3-ol, 9CI O-80025

Updated Entry replacing O-00469

[818-72-4]



(*S*)-*form*

(S)-form [32556-71-1]

Oil. Bp_{20} 88-89°. $[\alpha]_D^{20}$ −6.79° ($CHCl_3$).

(±)-form

Bp_{19} 83°.

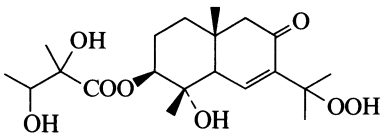
Midland, M.M., *J. Org. Chem.*, 1975, **40**, 2250 (*synth*)

Amos, R.A. *et al*, *J. Org. Chem.*, 1978, **43**, 555 (*synth*)

Larock, R.C. *et al*, *Tetrahedron*, 1987, **43**, 2013 (*resoln, pmr*)

Odonticin O-80026

[122398-17-8]



$C_{20}H_{32}O_8$ M 400.468

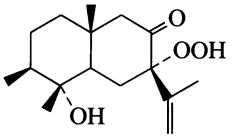
Constit. of *Pluchea arguta*. Syrup. $[\alpha]_D^{20}$ +178° (c, 0.01 in MeOH).

Ahmad, V.U. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 861 (*isol, pmr*)

Odontin O-80027

7α-Hydroperoxy-3β,4α-dihydroxy-11-eudesmen-8-one

[122398-16-7]



$C_{15}H_{24}O_5$ M 284.352

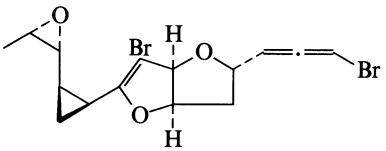
Constit. of *Pluchea arguta*. Gum. $[\alpha]_D^{20}$ −180° (c, 0.04 in MeOH).

Ahmad, V.U. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 561 (*isol, pmr*)

Okamurallene O-80028

Updated Entry replacing O-10035

[80539-33-9]



$C_{15}H_{16}Br_2O_3$ M 404.098

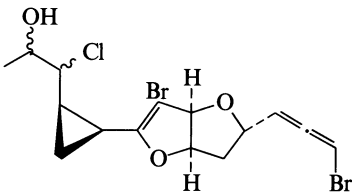
Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{26}$ +160° (c, 1.74 in $CHCl_3$).

Suzuki, M. *et al*, *Tetrahedron Lett.*, 1981, **22**, 3853 (*isol*)

Suzuki, M. *et al*, *Phytochemistry*, 1989, **28**, 2145 (*cmr, struct*)

Okamurallene chlorohydrin O-80029

[123297-19-8]



$C_{15}H_{17}Br_2ClO_3$ M 440.558

Metab. of *Laurencia intricata*. Cryst. (hexane). Mp 71-72°. $[\alpha]_D^{18}$ +205° (c, 0.325 in CCl_4).

Suzuki, M. *et al*, *Phytochemistry*, 1989, **28**, 2145 (*isol, pmr, cmr*)

11,13(18)-Oleanadiene-3,24-diol O-80030

$C_{30}H_{48}O_2$ M 440.708

3β-form [119285-49-3]

Constit. of *Phyllanthus flexuosus*. Needles ($MeOH/CHCl_3$). Mp 302-305°.

Tanaka, R. *et al*, *Phytochemistry*, 1988, **27**, 3563.

12-Oleanene-3,15-diol O-80031

$C_{30}H_{50}O_2$ M 442.724

(3β,15α)-form [61497-68-5]

Constit. of *Phyllanthus flexuosus*. Needles ($MeOH/CHCl_3$). Mp 245-246.5°. $[\alpha]_D^{23}$ +82.5° (c, 1.21 in $CHCl_3$).

Hui, W.H. *et al*, *Phytochemistry*, 1977, **15**, 1313 (*synth*)

Tanaka, R. *et al*, *Phytochemistry*, 1988, **27**, 3563 (*isol*)

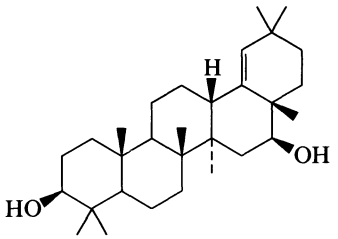
12-Oleanene-3,24-diol O-80032

$C_{30}H_{50}O_2$ M 442.724

3β-form [119318-15-9]
Constit. of *Phyllanthus flexuosus*. Needles (MeOH/$CHCl_3$). Mp 251-253°. $[\alpha]_D^{23}$ +84.7° (c, 0.46 in $CHCl_3$).

Ogihara, K. *et al*, *Phytochemistry*, 1987, **26**, 783 (*synth*)
Tanaka, R. *et al*, *Phytochemistry*, 1988, **27**, 3563 (*isol*)

18-Oleanene-3,16-diol O-80033



$C_{30}H_{50}O_2$ M 442.724

(3β,16β)-form [122577-94-0]
Constit. of *Schaefferia cuneifolia*. Cryst. Mp 237-238°. $[\alpha]_D^{20}$ +8.5° (c, 0.07 in $CHCl_3$).

Di-Ac: [122577-95-1].
$C_{34}H_{54}O_4$ M 526.798
Constit. of *S. cuneifolia*. Cryst. (EtOAc/hexane). Mp 230-232°. $[\alpha]_D^{20}$ +6.35° (c, 0.236 in $CHCl_3$).

3-Ketone: [122577-96-2]. *16β-Hydroxy-18-oleanen-3-one*
$C_{30}H_{48}O_2$ M 440.708
Occurs in *S. cuneifolia* as inseparable mixture with 16α-hydroxy-18-oleanen-3-one.

Gonzalez, A.G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 567 (*isol, pmr, cmr*)

12-Oleanene-3,16,21,22,23,28-hexol O-80034

Updated Entry replacing O-00508

$C_{30}H_{50}O_6$ M 506.721

(3β,16β,21β,22α)-form [22467-07-8] ***Gymnemagenin***
Aglycone from *Gymnema sylvestre*. Cryst. ($CHCl_3$/MeOH). Mp 328-335°. $[\alpha]_D^{25}$ +53.1° (c, 1 in MeOH).

3-O-β-D-Glucuronopyranosyl: Deacylgymnemic acid
Cryst. Mp 230-235°.

3-O-β-D-Glucuropyranosyl, 21-O-tigloyl: ***Gymnemic acid IV***
$C_{41}H_{64}O_{13}$ M 764.949
Constit. of *G. sylvestre*. Antisweet compound. Cryst. Mp 220-221° (213-215°). $[\alpha]_D$ +8.8° (c, 5.4 in MeOH).

3-O-β-Glucuronopyranosyl, 21-O-tigloyl, 28-Ac: ***Gymnemic acid I***
$C_{43}H_{66}O_{14}$ M 806.986
Constit. of *G. sylvestre*. Antisweet compound. Cryst. Mp 211-212°. $[\alpha]_D$ +36.7° (c, 2.4 in MeOH).

3-O-β-D-Glucuropyranosyl, 21-O-(2-methylbutanoyl): ***Gymnemic acid III***
$C_{41}H_{66}O_{13}$ M 766.965
Constit. of *G. sylvestre*. Antisweet compound. Mp 218-219° (209.5-212°). $[\alpha]_D$ +7.6° (c, 2.9 in MeOH).

3-O-β-D-Glucuronopyranosyl, 21-O-(S-2-methylbutanoyl), 28-Ac: ***Gymnemic acid II***
$C_{43}H_{68}O_{14}$ M 809.002
Constit. of *G. sylvestre*. Antisweet compound. Cryst. Mp 212-213°. $[\alpha]_D$ +36.3° (c, 1.5 in MeOH).

Subba Rao, G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 1681 (*struct*)
Hoge, R. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 1435 (*cryst struct*)
Yoshikawa, K. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1103 (*isol*)
Maeda, M. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1547 (*isol*)

12-Oleanene-3,16,21,23,28-pentol O-80035

Updated Entry replacing O-50037

3,16,21,23,28-Pentahydroxy-12-oleanene
$C_{30}H_{50}O_5$ M 490.722

(3β,16β,21β)-form [19942-02-0] ***Gymnestrogenin***
Constit. of *Gymnema sylvestre*. Cryst. Mp 288-289°. $[\alpha]_D^{24}$ +53.5° (c, 0.71 in MeOH).

16-Benzoyl: Cryst. ($CHCl_3$/MeOH). Mp 282-284°. $[\alpha]_D$ +59° (c, 1 in EtOH).

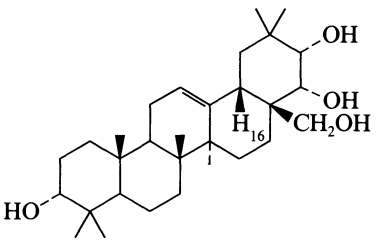
3-O-β-D-Glucopyranosyl-(1→3)-α-L-arabinopyranoside, 16-benzoyl: [107110-06-5]. ***Glochidioside***
$C_{48}H_{72}O_{15}$ M 889.088
Constit. of *Glochidion heyneanum*. Amorph. powder. $[\alpha]_D$ +42° (c, 1 in EtOH).

3-O-β-D-Glucopyranoside, 16-benzoyl: ***Glochidioside N***
$C_{43}H_{64}O_{11}$ M 756.972
Constit. of *G. heyneanum*. Amorph. powder.

3-O-(β-D-Glycopyranosyl-(1→2)-β-D-glucopyranoside), 16-benzoyl: ***Glochidioside Q***
$C_{49}H_{74}O_{16}$ M 919.114
Constit. of *G. heyneanum*. Amorph. powder.

Stocklin, W., *Helv. Chim. Acta*, 1968, **51**, 1235 (*isol*)
Srivastava, R. *et al*, *Phytochemistry*, 1986, **25**, 2672; 1988, **27**, 3575 (*derivs*)

12-Oleanene-3,21,22,28-tetrol O-80036



$C_{30}H_{50}O_4$ M 474.723

(3α,21α,22α)-form
Cryst. Mp 304°.

28-β-D-Xylopyranoside:
$C_{35}H_{58}O_8$ M 606.838
Constit. of *Centipeda minima*. Cryst. Mp 126°.

16α-Hydroxy: 12-Oleanene-3α,16α,21α,22α,28-pentol.
3α,16α,21α,22α,28-Pentahydroxy-12-oleanene
$C_{30}H_{50}O_5$ M 490.722
Cryst. Mp 315°.

16α-Hydroxy, 28-β-D-xylopyranoside:
$C_{35}H_{58}O_9$ M 622.838
Constit. of *C. minima*. Cryst. Mp 145°.

Gupta, D. *et al*, *Phytochemistry*, 1989, **28**, 1197.

12-Oleanene-2,3,23-triol O-80037

$C_{30}H_{50}O_3$ M 458.723

(2α,3β)-form
Constit. of *Commiphora merkeri*. Shows antiflammatory and analgesic properties. Needles. Mp 256°. $[\alpha]_D^{22}$ +48° (c, 1.8 in dioxan).

Fourie, T.G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1128 (*isol, pmr, cmr*)

12-Oleanene-3,15,24-triol O-80038

$C_{30}H_{50}O_3$ M 458.723

(3β,15α)-form [119285-50-6]

Constit. of *Phyllanthus flexuosus*. Needles. Mp 251-253°. $[\alpha]_D^{23}$ +59.9° (c, 0.58 in Py).

Tanaka, R. *et al*, *Phytochemistry*, 1988, **27**, 3563.

12-Oleanene-3,9,11-triol O-80039

$C_{30}H_{50}O_3$ M 458.723

(3β,9α,11α)-form

Constit. of *Euphorbia supina*. Cryst. ($MeOH/CHCl_3$). Mp 242-244°. $[\alpha]_D^{23}$ −11° (c, 0.33 in $CHCl_3$).

Tanaka, R. *et al*, *Phytochemistry*, 1989, **28**, 1699.

13(18)-Oleanene-3,22,24-triol O-80040

Updated Entry replacing S-00535

$C_{30}H_{50}O_3$ M 458.723

(3β,22α)-form

O^{22}-*Me:* [65892-76-4]. *22α-Methoxy-*13(18)*-oleanen-3β,24-diol.* ***Soyasapogenol D.*** *Soyasapogenol* M_3

$C_{31}H_{52}O_3$ M 472.750

Soya-bean saponin (from *Glycine max*). Probably an artifact. Cryst. ($Me_2CO/MeOH$). Mp 298-299°. $[\alpha]_D^{31}$ −60.8° ($CHCl_3$). Shown to be 21- or 22-methoxy by Cainelli *et al*. CA uses the 21-methoxy struct. but themost recent assignment seems to be that of Růzička.

Meyer, A. *et al*, *Helv. Chim. Acta*, 1950, **33**, 687 (*isol*)
Cainelli, G. *et al*, *Helv. Chim. Acta*, 1958, **41**, 2053 (*struct*)
Ružička, L., *Pure Appl. Chem.*, 1963, **6**, 505 (*struct, biosynth*)
Jurzysta, M. *et al*, *J. Chromatogr.*, 1978, **148**, 517 (*isol*)

18-Oleanen-3-ol O-80041

$C_{30}H_{50}O$ M 426.724

3β-form

Me ether: [5945-45-9]. *3β-Methoxy-*18*-oleanene.* ***Miliacin.*** *Prosol. Panicol*

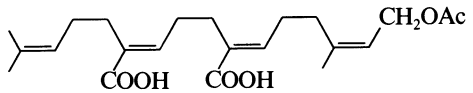
$C_{31}H_{52}O$ M 440.751

Isol. from millet (*Panicum miliaceum*), various *Chionochloa* spp. and other spp. in the Gramineae. Cryst. ($CHCl_3$). Mp 282-283°. $[\alpha]_D^{20}$ +22° (c, 0.88 in $CHCl_3$) (+8°).

Sugiyama, N. *et al*, *Nippon Kagaku Zasshi* (*Jpn. J. Chem.*), 1961, **82**, 1051, 1054, 1057; *CA*, **57**, 13810n (*isol, struct*)
Bryce, T.A. *et al*, *Tetrahedron*, 1967, **23**, 1283 (*ms*)
Russell, G.B. *et al*, *Phytochemistry*, 1976, **15**, 1933 (*isol*)

Oleaxillaric acid O-80042

[116139-49-2]

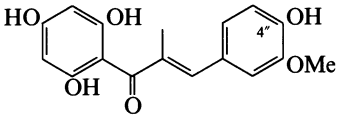


$C_{22}H_{32}O_6$ M 392.491

Constit. of *Olearia axillaris*.

Warning, U. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 513.

Olivin O-80043



$C_{17}H_{16}O_6$ M 316.310

Isol. from leaves of *Olea europaea*. Cryst. (EtOH/EtOAc). Mp >300°.

4''-O-(Glucosylglucoside): Olivin 4-diglucoside

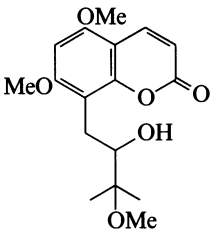
$C_{29}H_{36}O_{16}$ M 640.594

Isol. from *O. europaea*. Cryst. (MeOH aq.). Mp 220-225°. $[\alpha]_D^{20}$ −61.7° (Py).

Bočková, H. *et al*, *Collect. Czech. Chem. Commun.*, 1964, **29**, 1484 (*isol, uv, ir, struct*)

Omphalocarpin O-80044

[120693-45-0]



$C_{17}H_{22}O_6$ M 322.357

Constit. of *Murraya paniculata*. Needles ($CHCl_3/Me_2CO$). Mp 159-160°. $[\alpha]_D$ −44.1° (c, 0.3 in $CHCl_3$).

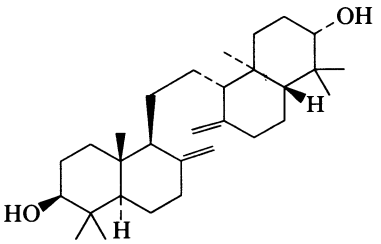
Wu, T.-S. *et al*, *Phytochemistry*, 1989, **28**, 293.

α-Onocerol O-80045

Updated Entry replacing O-10050

8(26),14(27)-Onceradiene-3β,21α-diol. α-Onocerin

[511-01-3]

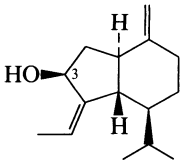


$C_{30}H_{50}O_2$ M 442.724

Constit. of *Ononis spinosa*, *O. arvensis*, *O. hircina* and *Lycopodium clavatum*. Cryst. (EtOH). Mp 232°. $[\alpha]_D$ +1° (Py), $[\alpha]_D^{20}$ +18° ($CHCl_3$).

Barton, D.H.R. *et al*, *J. Chem. Soc.*, 1955, 2639 (*isol, struct*)
Ageta, H. *et al*, *Chem. Pharm. Bull.*, 1962, **10**, 637 (*isol*)
Stork, G. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 3419 (*synth*)
Danieli, N. *et al*, *Tetrahedron*, 1967, **23**, 509 (*synth*)
Rowan, M.G. *et al*, *FEBS Lett.*, 1971, **12**, 229 (*biosynth*)
Tsuda, Y. *et al*, *Chem. Pharm. Bull.*, 1981, **29**, 3424 (*synth*)

4,10(14)-Oplopadien-3-ol O-80046



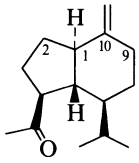
$C_{15}H_{24}O$ M 220.354
Biogenetic numbering (cf. cadinanes). Constit. of *Senecio mexicanus*. Cryst. Mp 54-56°. $[\alpha]_D$ +29° (c, 0.1 in $CHCl_3$).

3-Ketone: ***4(10),14-Oplopadien-3-one***
Constit. of *S. mexicanus*. Cryst. Mp 51-53°. $[\alpha]_D$ −194° (c, 2 in $CHCl_3$).

Joseph-Nathan, P. *et al*, *Phytochemistry*, 1989, **28**, 1207, 2397 (*isol, pmr, cmr, cryst struct*)

Oplopenone O-80047

Updated Entry replacing O-50045
Anhydrooplopanone
[28305-60-4]



$C_{15}H_{24}O$ M 220.354
Different numbering system used in references. Cadinane system used here. Constit. of *Euryops pedunculatus*. Cryst. (pet. ether). Mp 68°. $[\alpha]_D^{24}$ −15.2° (c, 0.4 in $CHCl_3$).

2α-Angeloyloxy: [119285-27-7]. *2α-Angeloxyanhydrooplopanone*. *1α-Angeloxyanhydrooplopanone* (*incorr.*)
$C_{20}H_{30}O_3$ M 318.455
Constit. of *Ambrosia artemisioides*. Oil.

$\Delta^{1,10}$*-Isomer, 2-oxo:* [119285-28-8]. *2-Oxoisoanhydrooplopanone*. *1-Oxoisoanhydrooplopanone* (*incorr.*)
$C_{15}H_{22}O_2$ M 234.338
Constit. of *A. artemisioides*. Oil.

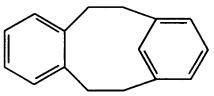
$\Delta^{1,10}$*-Isomer, 2α-angeloyloxy, 9-oxo:* [119285-29-9]. *2α-Angeloyloxy-9-oxoisoanhydrooplopanone*. *1α-Angeloyloxy-7-oxoisoanhydrooplopanone* (*incorr.*)
$C_{20}H_{28}O_4$ M 332.439
Constit. of *A. artemisioides*. Oil.

$\Delta^{1,10}$*-Isomer, 2α-cinnamoyloxy, 9-oxo:* [119285-30-2]. *2α-Cinnamoyloxy-9-oxoisoanhydrooplopanone*. *1α-Cinnamoyloxy-7-oxoisoanhydrooplopanone* (*incorr.*)
$C_{24}H_{28}O_4$ M 380.483
Constit. of *A. artemisioides*. Oil.

$\Delta^{1,10}$*-Isomer, 2α-anisoyloxy, 9-oxo:* [119285-31-3]. *2α-Anisoyloxy-9-oxoisoanhydrooplopanone*. *1α-Anisoyloxy-7-oxoisoanhydrooplopanone* (*incorr.*)
$C_{23}H_{28}O_5$ M 384.471
Constit. of *A. artemisioides*. Oil.

Bohlmann, F. *et al*, *Phytochemistry*, 1978, **17**, 1135 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3551 (*derivs*)

[2.2]Orthometacyclophane O-80048

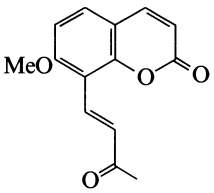


$C_{12}H_{12}$ M 156.227
Obt. as *syn-anti*-mixt.
[119392-52-8, 119477-47-3]

Bodwell, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 455 (*synth, pmr, cmr*)

Osthenone O-80049

[112789-90-9]

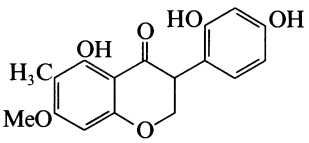


$C_{14}H_{12}O_4$ M 244.246
Constit. of *Citrus* spp. Yellow prisms. Mp 141-142°.

Ju-ichi, M. *et al*, *Heterocycles*, 1988, **27**, 2197.

Ougenin O-80050

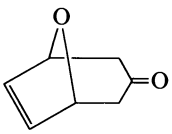
*3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5-hydroxy-7-methoxy-6-methyl-4*H*-1-benzopyran-4-one*. *2′,4′,5-Trihydroxy-7-methoxy-6-methylisoflavanone*
[1236-43-7]



$C_{17}H_{16}O_6$ M 316.310
Isol. from *Ougeinia dalbergioides*. Pale-yellow needles (EtOAc/pet. ether). Mp 239-241°.

Balakrishna, S.J.D. *et al*, *Proc. R. Soc. London, A*, 1962, **268**, 1.
Ahluwalia, V.K. *et al*, *Indian J. Chem.*, 1966, **4**, 250 (*isol*)

8-Oxabicyclo[3.2.1]oct-6-en-3-one O-80051

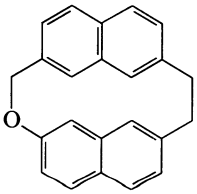


$C_7H_8O_2$ M 124.139
Oil, cryst. on standing. Mp 38°. Bp_{11} 110-130° (kugelrohr)

Föhlisch, B. *et al*, *Chem. Ber.*, 1988, **121**, 1585 (*synth, pmr, cmr*)

1-Oxa[2.2](2,7)naphthalenophane O-80052

2-Oxapentacyclo[11.5.3.3^{4,10}*.0*^{7,23}*0*^{16,20}*]tetracosa-1(19),4,6,8,10(22),13,15,17,20,23-decaene, 9CI*



$C_{23}H_{18}O$ M 310.395

(+)-*form* [118797-89-0]
$[\alpha]_{365}$ +72° (c, 0.79 in 1-butanol).

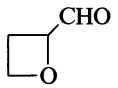
(−)-*form* [118797-90-3]
$[\alpha]_{365}$ −102.4° (c, 0.41 in $CHCl_3$).

(±)-*form* [118797-88-9]
Needles (hexane). Mp 206-208°.

Billen, S. *et al*, *Chem. Ber.*, 1989, **122**, 1113 (*synth, pmr, cmr, uv, cd*)

2-Oxetanecarboxaldehyde O-80053

2-Formyloxetane



$C_4H_6O_2$ M 86.090

(±)-*form*

2,4-Dinitrophenylhydrazone: Orange needles (Me_2CO). Mp 234-235°.

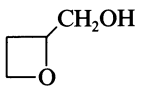
Di-Et acetal: 2-(Diethoxymethyl)oxetane
$C_8H_{16}O_3$ M 160.213
Liq. Bp_{10} 88-90°.

Fitton, A.O. *et al*, *Synthesis*, 1987, 1140 (*synth, ir, pmr*)

2-Oxetanemethanol, 9CI O-80054

2-Hydroxymethyloxetane

[61266-70-4]



$C_4H_8O_2$ M 88.106

(±)-*form* [84921-88-0]
Liq. Bp_{15} 94-98°.

4-Methylbenzenesulfonyl: Solid. Mp 58-59°.

Fitton, A.O. *et al*, *Synthesis*, 1987, 1140 (*synth, ir, pmr*)

3-Oxetanemethanol, 9CI O-80055

3-Hydroxymethyloxetane

[6246-06-6]

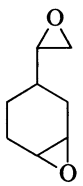
$C_4H_8O_2$ M 88.106

U.S. Pat., 3 301 923, (1967); *CA*, **66**, 67673c.

3-Oxiranyl-7-oxabicyclo[4.1.0]heptane, 9CI O-80056

3-(Epoxyethyl)-7-oxabicyclo[4.1.0]heptane, 8CI. 1,2-Epoxy-4-(epoxyethyl)cyclohexane. 1-Epoxyethyl-3,4-epoxycyclohexane. 4-Vinylcyclohexene dioxide

[106-87-6]



$C_8H_{12}O_2$ M 140.182

Coml. samples are presumably mixts. of diastereoisomers. Used to make water-resistant adhesives, corrosion inhibitors and polymer stabilizers; cross-linking agent; ingredient in rocket fuels. Liq. V. sol. H_2O. d_{20}^{20} 1.099. Mp < −55°. Bp 227°, Bp_5 88-92°. n_D^{27} 1.476.

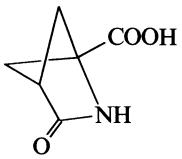
▷ Mutagenic. Carcinogenic, toxic to ovaries.

Everett, J.L. *et al*, *J. Chem. Soc.*, 1950, 3131 (*synth*)
Kodama, J.K. *et al*, *Arch. Environ. Health*, 1961, **2**, 50; *ca*, **55**, 13687i (*tox*)
Watabe, T. *et al*, *Biochem. Pharmacol.*, 1976, **25**, 601 (*metab*)
Fr. Pat., 2 393 799, (1979); *ca*, **91**, 158325y (*manuf*)
Turchi, G. *et al*, *Mutat. Res.*, 1981, **83**, 419; *ca*, **96**, 1577n (*tox*)
Bloch, R. *et al*, *J. Org. Chem.*, 1985, **50**, 1544 (*synth*)
Maronpot, R.R., *EHP Environ. Health Perspect.*, 1987, **13**, 125; *ca*, **107**, 213022y (*rev, bibl, tox*)

3-Oxo-2-azabicyclo[2.1.1]hexane-1-carboxylic acid, 9CI O-80057

2,4-Methanopyroglutamic acid

[116128-98-4]



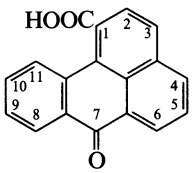
$C_6H_7NO_3$ M 141.126
Unstable.

Me ester: [116129-05-6].
$C_7H_9NO_3$ M 155.153
Cryst. Mp 76.5-77.5°.

Hughes, P. *et al*, *J. Org. Chem.*, 1988, **53**, 4793 (*synth, pmr, cmr, ms, ir*)

7-Oxo-7*H*-benz[*de*]anthracene-1-carboxylic acid, 9CI, 8CI O-80058

Benzanthrone-1-carboxylic acid



$C_{18}H_{10}O_3$ M 274.275
Cryst. ($PhNO_2$). Mp 285°.

Boyes, W.H.D. *et al*, *J. Chem. Soc.*, 1938, 1833 (*synth*)

7-Oxo-7*H*-benz[*de*]anthracene-2-carboxylic acid, 9CI, 8CI O-80059

Benzanthrone-2-carboxylic acid

$C_{18}H_{10}O_3$ M 274.275
Yellow needles ($PhNO_2$). Mp 348-349°.

Et ester:
$C_{20}H_{14}O_3$ M 302.329
Yellow cryst. (EtOH). Mp 172-173°.

Chloride:
$C_{18}H_9ClO_2$ M 292.721
Yellow prisms (chlorobenzene). Mp 252-253°.

Amide:
$C_{18}H_{11}NO_2$ M 273.290
Cryst. ($PhNO_2$). Mp 306°.

Nitrile: 2-Cyanobenzanthrone
$C_{18}H_9NO$ M 255.275
Yellow cryst. ($PhNO_2$). Mp 285-286°.

Heilbron, I.M. *et al*, *J. Chem. Soc.*, 1936, 781 (*nitrile, amide*)
Baddar, F.G. *et al*, *J. Chem. Soc.*, 1941, 310 (*synth*)
Vollmann, H., *Justus Liebigs Ann. Chem.*, 1963, **669**, 22 (*chloride*)

7-Oxo-7*H*-benz[*de*]anthracene-3-carboxylic acid, 9CI, 8CI **O-80060**

Benzanthrone-3-carboxylic acid

[67971-99-7]

$C_{18}H_{10}O_3$ M 274.275
Yellow needles ($PhNO_2$). Mp 343-344°.

Chloride:
$C_{18}H_9ClO_2$ M 292.721
Golden yellow needles. Mp 260-261°.

Nitrile: 3-Cyanobenzanthrone
$C_{18}H_9NO$ M 255.275
Yellow cryst. ($PhNO_2$). Mp 242-243°.

Heilbron, I.M. *et al*, *J. Chem. Soc.*, 1936, 781 (*nitrile*)
Vollmann, H., *Justus Liebigs Ann. Chem.*, 1963, **669**, 22 (*synth, chloride*)
Gorelik, M.V. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1978, **14**, 1433; 1979, **15**, 2322 (*synth*)

7-Oxo-7*H*-benz[*de*]anthracene-4-carboxylic acid, 9CI, 8CI **O-80061**

Benzanthrone-4-carboxylic acid

$C_{18}H_{10}O_3$ M 274.275
Yellow cryst. ($PhNO_2$). Mp 314-315°.

Me ester:
$C_{19}H_{12}O_3$ M 288.302
Yellow cryst. (MeOH). Mp 215-216°.

Et ester:
$C_{20}H_{14}O_3$ M 302.329
Yellow cryst. (EtOH). Mp 134-135°.

Nitrile: 4-Cyanobenzanthrone
$C_{18}H_9NO$ M 255.275
Yellow cryst. ($PhNO_2$). Mp 234°.

U.S. Pat., 1 874 547, (1928) (*nitrile*)
Copp, F.C. *et al*, *J. Chem. Soc.*, 1942, 209 (*synth*)

7-Oxo-7*H*-benz[*de*]anthracene-8-carboxylic acid, 9CI, 8CI **O-80062**

Benzanthrone-8-carboxylic acid

[73975-18-5]

$C_{18}H_{10}O_3$ M 274.275
Yellow cryst. (chlorobenzene). Mp 262-263°. Tautomerises to cyclic hydroxylactone.

Me ester:
$C_{19}H_{12}O_3$ M 288.302
Yellow cryst. (MeOH/MeOAc). Mp 173.5-174.5°.

Copp, F.C. *et al*, *J. Chem. Soc.*, 1942, 209 (*synth*)
Baddar, F.G. *et al*, *J. Chem. Soc.*, 1944, 450 (*synth*)
Gomès, L.M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1980, **290**, 29 (*synth, ir*)

7-Oxo-7*H*-benz[*de*]anthracene-9-carboxylic acid, 9CI, 8CI **O-80063**

Benzanthrone-9-carboxylic acid

$C_{18}H_{10}O_3$ M 274.275
Yellow cryst. ($PhNO_2$). Mp 352-354°.

Me ester:
$C_{19}H_{12}O_3$ M 288.302
Yellow cryst. (MeOH). Mp 188-189°.

Et ester:
$C_{20}H_{14}O_3$ M 302.329
Yellow cryst. (EtOH). Mp 172.5-173.5°.

Copp, F.C. *et al*, *J. Chem. Soc.*, 1942, 209 (*synth*)

7-Oxo-7*H*-benz[*de*]anthracene-10-carboxylic acid, 9CI, 8CI **O-80064**

Benzanthrone-10-carboxylic acid

$C_{18}H_{10}O_3$ M 274.275
Yellow cryst. ($PhNO_2$). Mp 326-327°.

Me ester:
$C_{19}H_{12}O_3$ M 288.302
Yellow cryst. (MeOH). Mp 168-169°.

Et ester:
$C_{20}H_{14}O_3$ M 302.329
Yellow-gold cryst. (EtOH). Mp 136-138°.

Copp, F.C. *et al*, *J. Chem. Soc.*, 1942, 209.
Bachmann, W.E. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 3062.

7-Oxo-7*H*-benz[*de*]anthracene-11-carboxylic acid, 9CI, 8CI **O-80065**

Benzanthrone-11-carboxylic acid

$C_{18}H_{10}O_3$ M 274.275
Yellow cryst. (EtOH). Mp 273°.

Me ester:
$C_{19}H_{12}O_3$ M 288.302
Yellow cryst. (MeOH). Mp 160-161°.

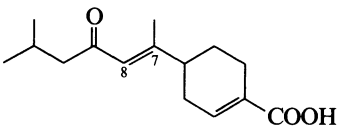
Amide:
$C_{18}H_{11}NO_2$ M 273.290
Yellow cryst. ($PhNO_2$). Mp 325-327°.

Rull, H.G. *et al*, *J. Chem. Soc.*, 1935, 571; 1937, 1096 (*synth*)
Bigelow, L.A. *et al*, *J. Chem. Soc.*, 1935, 573 (*synth*)
Boyes, W.H.D. *et al*, *J. Chem. Soc.*, 1938, 1833 (*amide*)
Copp, F.C. *et al*, *J. Chem. Soc.*, 1942, 209 (*synth, ester, amide*)
Craig, J.T. *et al*, *Aust. J. Chem.*, 1966, **19**, 1927 (*synth*)

9-Oxo-2,7-bisaboladien-15-oic acid **O-80066**

4-(1,5-Dimethyl-3-oxo-1-hexenyl)-1-cyclohexene-1-carboxylic acid, 9CI. ***Atlantonic acid***

[120019-19-4]



$C_{15}H_{22}O_3$ M 250.337
Constit. of *Cedrus libani*. Oil.

7,8-Dihydro: [120019-18-3]. *9-Oxo-2-bisabolen-15-oic acid.* ***Dihydroatlantonic acid***
$C_{15}H_{24}O_3$ M 252.353
Constit. of *C. libani*. Oil.

Avcibasi, H. *et al*, *Phytochemistry*, 1988, **27**, 3967.

2-Oxobutanal, 9CI **O-80067**

2-Oxobutyraldehyde, 8CI. Ethylglyoxal

[4417-81-6]

H_3CCH_2COCHO

$C_4H_6O_2$ M 86.090
Liq. Sol. H_2O. Bp 90°. n_D^{25} 1.4006.

1-Oxime:
$C_4H_7NO_2$ M 101.105
Hygroscopic needles (C_6H_6). Mp 55°.

Bis(2,4-dinitrophenylhydrazone): [1179-34-6].
Red needles (C_6H_6). Mp 247°.

Di-Me acetal: [6342-57-0]. *1,1-Dimethoxy-2-butanone*
$C_6H_{12}O_3$ M 132.159
Liq. Bp 125-128°, Bp_{13} 49°.

Di-Et acetal: 1,1-Diethoxy-2-butanone

$C_8H_{16}O_3$ M 160.213
Liq. Bp_{55} 98-100°. n_D^{20} 1.408.

Riley, R. *et al*, *J. Chem. Soc.*, 1932, 1877 (*synth*)
Ingold, C.K. *et al*, *J. Chem. Soc.*, 1934, 85 (*synth*)
Sharp, W. *et al*, *J. Chem. Soc.*, 1948, 1863 (*oxime*)
Royals, E.E. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 4161 (*synth*)
Dulou, R. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1966, **262**, 564 (*acetal*)

4-Oxobutanoic acid, 9CI O-80068

Updated Entry replacing O-00777
Succinaldehydic acid, 8CI. Succinic semialdehyde. 3-Formylpropionic acid. γ-Oxobutanoic acid
[692-29-5]

$OHCCH_2CH_2COOH$

$C_4H_6O_3$ M 102.090
Found in *Proteus vulgaris*, and in mouse brains. Has anaesthetic props. Oil with rancid odour. Sol. H_2O, EtOH, Et_2O, C_6H_6. Bp_{14} 134-136°. Steam-volatile.

▷ Mod. toxic. Emits toxic fumes on contact with acids or heating to dec.. WM3380000.

Trimer: [26817-25-4]. s-*Trioxane*-2,4,6-*tripropionic acid.* 1,3,5-*Tris*-(*β-carboxyethyl*)-s-*trioxane*
$C_{12}H_{18}O_9$ M 306.269
Prisms. Sl. sol. Et_2O, EtOAc, aq. Na_2CO_3. Mp 147°. Bp_{14} 134-136°. On dist. → monomer.

Me ester: [13865-19-5].
$C_5H_8O_3$ M 116.116
Oil. Bp_{15} 69-71°.

Me ester, semicarbazone: Cryst. Mp 130-131°.

Me ester, 2,4-dinitrophenylhydrazone: Cryst. Mp 131-132°.

Nitrile: [3515-93-3]. *4-Oxobutanenitrile, 9CI. Succinaldehydonitrile, 8CI.* 3-*Cyanopropanal*
C_4H_5NO M 83.090
Bp 77°.

Oxime:
$C_4H_7NO_3$ M 117.104
Cryst. (EtOH). Mp 102-103° (155°).

Semicarbazone: Prisms or needles (H_2O). Mp 190-191° dec.

2,4-Dinitrophenylhydrazone: [4093-65-6].
Yellow cryst. Mp 201°.

Nitrile, 2,4-dinitrophenylhydrazone: Mp 198-199°.

Nitrile, di-Me acetal: 4,4-Dimethoxybutanenitrile
$C_6H_{11}NO_2$ M 129.158
Bp_{20} 110°.

Nitrile, di-Et acetal: [18381-45-8]. *4,4-Diethoxybutanenitrile*
$C_8H_{15}NO_2$ M 157.212
Bp_{10} 97°.

Wislicenus, W. *et al*, *Justus Liebigs Ann. Chem.*, 1908, **363**, 340 (*synth, derivs*)
Kato, J. *et al*, *CA*, 1962, **57**, 2064 (*nitrile*)
Nawar, W.W. *et al*, *J. Agric. Food Chem.*, 1971, **19**, 1039 (*ester*)
Watanabe, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2490 (*synth*)
Doleschall, G., *Tetrahedron*, 1976, **32**, 2549 (*ester*)
Pirkle, W.H. *et al*, *J. Org. Chem.*, 1978, **43**, 2091 (*nitrile*)
Manzocchi, A. *et al*, *Synthesis*, 1983, 324 (*synth*)
Gannett, P.M. *et al*, *J. Org. Chem.*, 1988, **53**, 1064 (*Me ester, synth, ir, pmr, cmr, ms*)
Gribble, G.W. *et al*, *J. Org. Chem.*, 1988, **53**, 3164 (*nitrile di-Me acetal*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 664.

2-Oxo-3-butynoic acid, 9CI O-80069

[56842-75-2]

$HC{\equiv}CCOCOOH$

$C_4H_2O_3$ M 98.058
Unstable. Reactive alkylating agent *in vivo*.

▷ Possible mutagen.

Kaczorowski, G. *et al*, *Biochemistry*, 1975, **14**, 3903.
Pompon, D. *et al*, *Eur. J. Biol.*, 1982, **129**, 143 (*synth, purifn*)

4-Oxo-2-butynoic acid O-80070

$OHCC{\equiv}CCOOH$

$C_4H_2O_3$ M 98.058

Et ester: [78076-22-9].
$C_6H_6O_3$ M 126.112
Pale yellow liq. Bp_3 57-58°.

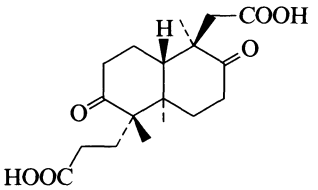
Dimethylamide: [104387-58-8].
$C_6H_7NO_2$ M 125.127
Liq.

Nitrile: [90108-94-4]. *4-Oxo-2-butynenitrile*
C_4HNO M 79.058
Pale yellow liq. Not obt. pure.

Barbot, F. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 313 (*synth*)
Epsztein, R. *et al*, *Bull. Soc. Chim. Fr., Part II*, 1983, 41 (*synth*)
Gorgues, A. *et al*, *Tetrahedron*, 1986, **42**, 351 (*synth, pmr, ir*)

3-Oxo-17-carboxy-3,18-secobarbacenic acid O-80071

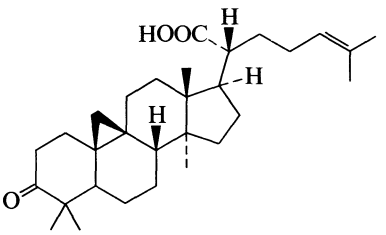
5-(Carboxymethyl)decahydro-1,5,8a-trimethyl-2,6-dioxo-1-naphthalenepropanoic acid, 9CI
[119967-65-6]



$C_{18}H_{26}O_6$ M 338.400
Constit. of *Barbacenia flava*. Cryst. (EtOAc/hexane). Mp 214-216°.

Pinto, A.C. *et al*, *Phytochemistry*, 1988, **27**, 3917.

3-Oxo-24-cycloarten-21-oic acid O-80072

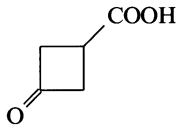


$C_{30}H_{46}O_3$ M 454.692
Constit. of leaves of *Lansium domesticum*. Skin tumour inhibitor. Cryst. Mp 185-186°. $[\alpha]_D^{12}$ +18.7° (c, 1.16 in $CHCl_3$).

Nishizawa, M. *et al*, *Tetrahedron Lett.*, 1989, **30**, 5615 (*cryst struct*)

3-Oxocyclobutanecarboxylic acid O-80073

[23761-23-1]



$C_5H_6O_3$ M 114.101
Needles (C_6H_6/hexane). Mp 69-70°.

N,N-*Dimethylamide:*
$C_7H_{11}NO_2$ M 141.169
Bp_1 108-111°.

N,N-*Dimethylamide, ethylene ketal:* Bp_1 114°.

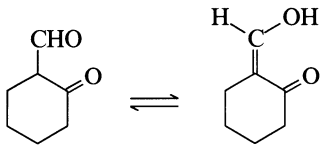
N,N-*Dimethylamide, Di-Et ketal:*
$C_{11}H_{21}NO_3$ M 215.292
Bp_1 110°.

Avram, M. *et al*, *Chem. Ber.*, 1957, **90**, 1424 (*deriv, synth*)
Caserio, F.F. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 5837 (*synth, deriv*)
Pigou, P.E. *et al*, *J. Org. Chem.*, 1988, **53**, 3841 (*synth, pmr, cmr*)

2-Oxocyclohexanecarboxaldehyde, 9CI, 8CI O-80074

2-(Hydroxymethylene)cyclohexanone, 9CI, 8CI. 2-Formylcyclohexanone

[823-45-0]



oxo-form *(Z-enol)-form*

$C_7H_{10}O_2$ M 126.155
(*Z*)-Enol form predominates. Liq. Bp_{14} 86-87°, Bp_5 70-72°. pK_a 6.35 (20°). n_D^{25} 1.5110. Polymerises slowly at r.t.

Me ether: [15839-18-6]. *2-(Methoxymethylene)cyclohexanone, 9CI*
$C_8H_{12}O_2$ M 140.182
Liq. Bp_{13} 75-80°, Bp_2 84-86°. n_D^{18} 1.4854.

[1193-63-1, 39695-64-2, 72036-60-3]

Garbisch, E.W., *J. Am. Chem. Soc.*, 1963, **85**, 1696; 1965, **87**, 505 (*tautom, pmr, cmr*)
Org. Synth., Coll. Vol., 4, 1963, 536 (*synth*)
Barna, J.C.J. *et al*, *Tetrahedron Lett.*, 1979, 1455 (*cmr, deriv*)
Brady, W.T. *et al*, *J. Org. Chem.*, 1983, **48**, 5337 (*synth, ir, pmr, deriv*)
Jones, R.A. *et al*, *Tetrahedron*, 1984, **40**, 1051 (*synth, tautom, ir, cmr*)

3-Oxocyclohexanecarboxaldehyde, 9CI, 8CI O-80075

3-Formylcyclohexanone

[69814-26-2]

$C_7H_{10}O_2$ M 126.155
Liq. Polymerises on heating.

Baisted, D.J. *et al*, *J. Chem. Soc.*, 1961, 4089 (*synth*)
Cohen, T. *et al*, *Tetrahedron Lett.*, 1978, 3533 (*synth*)
Lucchetti, A. *et al*, *Synth. Commun.*, 1983, **13**, 1153 (*synth*)
Ricci, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 1068 (*synth, ir*)
Kerdesky, F.A.J. *et al*, *J. Med. Chem.*, 1987, **30**, 1177 (*synth, pmr*)

4-Oxocyclohexanecarboxaldehyde, 9CI, 8CI O-80076

4-Formylcyclohexanone

[55882-00-3]

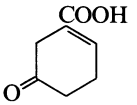
$C_7H_{10}O_2$ M 126.155
Liq. d_4^{20} 1.091. Bp_{10} 113-113.5°. n_D^{20} 1.4760.

Bissemicarbazone: Cryst. (MeOH). Mp 199°.

Petrov, A.A., *J. Gen. Chem. USSR* (*Engl. Transl.*), 1941, **11**, 661; *ca*, **36**, 1593 (*synth*)
Fetizon, M. *et al*, *Tetrahedron*, 1975, **31**, 171 (*synth*)

5-Oxo-1-cyclohexene-1-carboxylic acid O-80077

[37051-60-8]



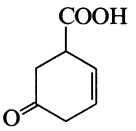
$C_7H_8O_3$ M 140.138
Cryst. (toluene). Mp 99-100°.

Me ester: [66838-90-2].
$C_8H_{10}O_3$ M 154.165
Liq. $Bp_{0.1}$ 80-83°.

Biffin, M.E.C. *et al*, *Aust. J. Chem.*, 1972, **25**, 1329 (*synth, ir, pmr*)
Webster, F.X. *et al*, *Synthesis*, 1987, 922 (*synth, pmr*)

5-Oxo-2-cyclohexene-1-carboxylic acid O-80078

[37051-56-2]



$C_7H_8O_3$ M 140.138

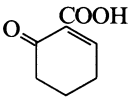
(±)-***form***
Cryst. (toluene). Mp 104-105°.

Me ester:
$C_8H_{10}O_3$ M 154.165
Bp_2 134-137°.

Me ester, 2,4-dinitrophenylhydrazone: Cryst. Mp 144-145°.

Biffin, M.E.C. *et al*, *Aust. J. Chem.*, 1972, **25**, 1329 (*synth, ir, pmr, deriv*)
Webster, F.X. *et al*, *Synthesis*, 1987, 922 (*synth, pmr*)

6-Oxo-1-cyclohexene-1-carboxylic acid O-80079



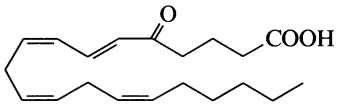
$C_7H_8O_3$ M 140.138

Me ester: [57039-20-0]. *2-Carbomethoxy-2-cyclohexen-1-one*
$C_8H_{10}O_3$ M 154.165
Undergoes Diels-Alder reacns. Liq.

Liotta, D. *et al*, *J. Org. Chem.*, 1981, **46**, 2920 (*synth*)
Liu, H.J. *et al*, *Can. J. Chem.*, 1988, **66**, 3143 (*use, ester*)

5-Oxo-6,8,11,14-eicosatetraenoic acid O-80080

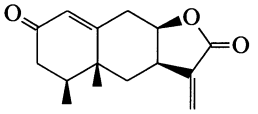
5-KETE



$C_{20}H_{30}O_3$ M 318.455

Toda, M. *et al*, *J. Med. Chem.*, 1983, **26**, 72 (*synth*)
Kerdesky, F.A.J. *et al*, *J. Med. Chem.*, 1987, **30**, 1177 (*synth, pmr*)

2-Oxo-1(10),11(13)-eremophiladien-12,8-olide O-80081



$C_{15}H_{18}O_3$ M 246.305

8β-form

Constit. of *Ondetia linearis*. Oil.

Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653.

4-Oxo-2-hexenoic acid, 8CI O-80082

[5636-58-8]

$H_3CCH_2COCH{=}CHCOOH$

$C_6H_8O_3$ M 128.127

(E)-form

Cryst. (pet. ether). Mp 109-110°.

Me ester: [90670-10-3].
$C_7H_{10}O_3$ M 142.154
Mp 30-32°. $Bp_{16.5}$ 80-81.5°.

Et ester: [61454-94-2].
$C_8H_{12}O_3$ M 156.181
$Bp_{11.5}$ 95-100°.

[70038-66-3, 83349-25-1]

Noltes, A.W. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1961, **80**, 1334 (*deriv*)
Reinheckel, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1966, **5**, 511 (*synth*)
Nakayama, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 184 (*deriv*)
Shnol, R.T. *et al*, *Zh. Obshch. Khim.*, 1982, **52**, 1351 (*Z-form*)
Miyashita, M. *et al*, *J. Org. Chem.*, 1984, **49**, 2857 (*deriv*)
Schuda, P.F. *et al*, *Synthesis*, 1987, 1055 (*deriv, synth, ir, pmr*)

5-Oxo-3-hexenoic acid, 8CI O-80083

[32794-12-0]

$H_3CCOCH{=}CHCH_2COOH$

$C_6H_8O_3$ M 128.127

(E)-form [28845-68-3]

Pale yellow oil.

2,4-Dinitrophenylhydrazone: Orange needles (EtOAc). Mp 177.5-178°.

Harris, T.M. *et al*, *J. Org. Chem.*, 1971, **36**, 2181 (*synth, nmr*)
Dieter, R.K. *et al*, *J. Org. Chem.*, 1988, **53**, 2031 (*synth, nmr*)

6-Oxo-4-hexenoic acid O-80084

[82934-89-2]

$OHCCH{=}CHCH_2CH_2COOH$

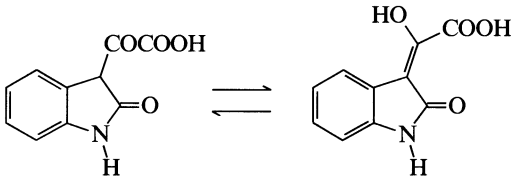
$C_6H_8O_3$ M 128.127

Maurer, B. *et al*, *Helv. Chim. Acta*, 1982, **65**, 462 (*synth, ir, nmr*)

2-Oxo-3-indolineglyoxylic acid O-80085

(1,2-Dihydro-2-oxo-3H-indol-3-ylidene)hydroxyacetic acid, 9CI. 3-Oxindolylglyoxylic acid

[14370-71-9]



$C_{10}H_7NO_4$ M 205.170

Completely enolised. Cryst. (Me_2CO). Mp 265° (256-257°).

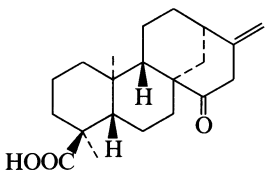
Et ester: [14370-70-8].
$C_{12}H_{11}NO_4$ M 233.223
Cryst. (Me_2CO). Mp 186-187°.

Benzyl ester: [110655-07-7].
$C_{17}H_{13}NO_4$ M 295.294
Yellow needles (Me_2CO). Mp 205-206°.

Wislicenus, W. *et al*, *Justus Liebigs Ann. Chem.*, 1924, **436**, 113 (*synth*)
Horner, L. *et al*, *Justus Liebigs Ann. Chem.*, 1941, **548**, 117 (*synth*)
Julian, P.L. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 5305 (*derivs*)
Harley-Mason, J. *et al*, *J. Chem. Soc.*, 1958, 3639 (*synth*)
Lewer, P., *J. Chem. Soc., Perkin Trans.* 1, 1987, 753 (*synth, pmr, uv, derivs*)

ent-15-Oxo-16-kauren-18-oic acid O-80086

[71493-37-3]



$C_{20}H_{28}O_3$ M 316.439

Constit. of *Croton argyrophylloides*. Cryst. (hexane/MeOH). Mp 202-204°. $[\alpha]_D^{25}$ −73° (c, 2.21 in $CHCl_3$).

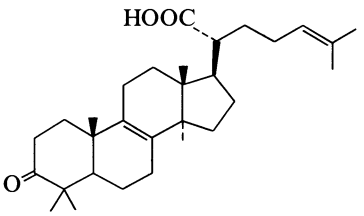
Monte, F.J.Q. *et al*, *Phytochemistry*, 1988, **27**, 3209.

3-Oxo-8,24-lanostadien-21-oic acid O-80087

Updated Entry replacing P-01917

Pinicolic acid A. α-Pinicolic acid

[466-05-7]



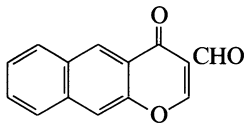
$C_{30}H_{46}O_3$ M 454.692

Produced by *Polyporus pinicola, Heterobasidion tasmanica* and *Fomes senex*. Cryst. Mp 205-207°. $[\alpha]_D$ +68° (c, 0.83 in $CHCl_3$).

Guider, J.M. *et al*, *J. Chem. Soc.*, 1954, 4471 (*isol*)
Batta, A.K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 451 (*isol, pmr*)

4-Oxo-4*H*-naphtho[2,3-*b*]pyran-3-carboxaldehyde **O-80088**

[57051-28-2]



$C_{14}H_8O_3$ M 224.215
Plates (EtOAc). Mp 222-224°.

Cremins, P.J. *et al*, *Tetrahedron*, 1987, **43**, 3075 (*synth, ir, pmr*)

5-Oxopentanoic acid, 9CI **O-80089**

Updated Entry replacing O-20065
4-Formylbutanoic acid. Glutaric semialdehyde
[5746-02-1]

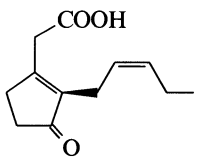
$OHCCH_2CH_2CH_2COOH$

$C_5H_8O_3$ M 116.116
Me ester: [6026-86-4].
$C_6H_{10}O_3$ M 130.143
Synthon. Liq. Bp_{10} 90-98°.
Nitrile: [3350-74-1]. *4-Cyanobutanal*
C_5H_7NO M 97.116
Liq. Bp_2 83-84°.
Nitrile, 2,4-dinitrophenylhydrazone: Mp 117-118°.

Brown, H.C. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 4606 (*nitrile, synth*)
Huckstep, M. *et al*, *Synthesis*, 1982, 881.
Gannett, P.M. *et al*, *J. Org. Chem.*, 1988, **53**, 1064 (*ester, synth, ir, pmr, cmr, ms*)
Bergeron, R.J. *et al*, *J. Org. Chem.*, 1988, **53**, 3131 (*nitrile, pmr, ir*)

3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid **O-80090**

3,7-Didehydrojasmonic acid

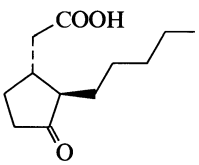


(Z)-form [120282-76-0]
$C_{12}H_{16}O_3$ M 208.257
Constit. of *Vicia faba*. Oil.

Miersch, O. *et al*, *Phytochemistry*, 1989, **28**, 339.

3-Oxo-2-pentylcyclopentaneacetic acid **O-80091**

9,10-Dihydrojasmonic acid
[98674-52-3]



$C_{12}H_{20}O_3$ M 212.288
Constit. of *Vicia faba*. Oil. $[\alpha]_D^{22}$ −28.3° (c, 0.1 in MeOH).
[76968-33-7]

Miersch, O. *et al*, *Phytochemistry*; 1989, **28**, 339.

3-Oxo-5-phenylpentanal **O-80092**

β-Oxobenzenepentanal, 9CI. 3-Oxo-5-phenylvaleraldehyde, 8CI

$PhCH_2CH_2COCH_2CHO$

$C_{11}H_{12}O_2$ M 176.215
Readily oligomerises, isol. as Cu chelate.
Cu chelate: Blue cryst. ($EtOH/CHCl_3$). Mp 176-178°.

Harris, T.M. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 3273 (*synth*)

4-Oxo-5-phenylpentanal **O-80093**

γ-Oxobenzenepentanal, 9CI. 4-Oxo-5-phenylvaleraldehyde, 8CI
[53707-97-4]

$PhCH_2COCH_2CH_2CHO$

$C_{11}H_{12}O_2$ M 176.215
Liq. $Bp_{0.02}$ 60-65°.

Brown, E. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 1001 (*synth, ir, pmr*)
Baldwin, S.W. *et al*, *Tetrahedron Lett.*, 1982, **23**, 3883 (*synth*)

5-Oxo-5-phenylpentanal **O-80094**

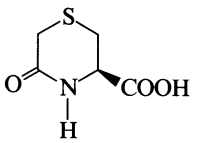
δ-Oxobenzenepentanal, 9CI. 5-Oxo-5-phenylvaleraldehyde, 8CI. 4-Benzoylbutyraldehyde
[75424-63-4]

$PhCOCH_2CH_2CH_2CHO$

$C_{11}H_{12}O_2$ M 176.215
Liq.
Di-Me acetal:
$C_{13}H_{16}O_2$ M 204.268
Oil.

Masahino, M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1980, 1950, 2909 (*synth, ir, pmr*)
Ounsworth, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 232 (*props*)

5-Oxo-3-thiomorpholinecarboxylic acid, 9CI **O-80095**

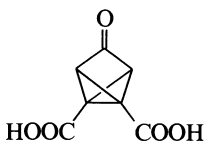


$C_5H_7NO_3S$ M 161.181
(R)-form
Oil.
Me ester: [118903-82-5].
$C_6H_9NO_3S$ M 175.208
Cryst. (Et_2O). Mp 70-71°. $[\alpha]_D$ −4.0° (c, 1.0 in $CHCl_3$).

Zanotti, G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2647 (*synth, ir, pmr*)

3-Oxotricyclo[2.1.0.0^{2,5}]pentane-1,5-dicarboxylic acid **O-80096**

[114534-19-9]



$C_7H_4O_5$ M 168.106

Solid. Mp *ca.* 170° dec. (discolours from 120°).

Di-Me ester: [81710-09-0].
$C_9H_8O_5$ M 196.159
Cryst. (CH_2Cl_2/hexane). Mp 130-131°.

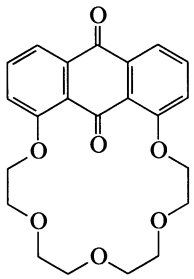
Di-Me ester, ethylene ketal: [114534-20-2].
$C_{11}H_{12}O_6$ M 240.212
Cryst. (Et_2O/pentane). Mp 83-86°.

Irngartinger, H. *et al*, *J. Org. Chem.*, 1988, **53**, 3046 (*synth, deriv, pmr, ir, ms*)

1,8-Oxybis(ethyleneoxyethyleneoxy)-9,10-anthracenedione O-80097

*6,7,9,10,12,13,15,16-Octahydro-1,21-methano-22*H-*dibenzo*[n,q][*1,4,7,10,13*]*pentaoxacyclooctadecin-22,23-dione, 9CI*

[111959-53-6]



$C_{22}H_{22}O_7$ M 398.412
Strong cation binder. Yellow cryst. solid (toluene). Mp 155-156°.

Delgado, M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 119 (*synth, esr, pmr, ir*)

3,3′-Oxybispropanoic acid O-80098

Bis(2-carboxyethyl)ether. Diethyl ether 2,2′-dicarboxylic acid

[5961-83-1]

$$HOOCCH_2CH_2OCH_2CH_2COOH$$

$C_6H_{10}O_5$ M 162.142
Cryst. (Me_2CO/pet. ether). Mp 60-61° (48-49°).

Di-Me ester:
$C_8H_{14}O_5$ M 190.196
Bp_3 90-91°.

Dichloride: [44995-78-0].
$C_6H_8Cl_2O_3$ M 199.033
Oil. Bp_1 85-88°.

Diamide:
$C_6H_{12}N_2O_3$ M 160.172
Mp 146°.

Dinitrile: Bis(2-cyanoethyl)ether
$C_6H_8N_2O$ M 124.142
Oil. d_{25}^{25} 1.05. Bp_5 161-162°.

Bruson, H.E., *J. Am. Chem. Soc.*, 1943, **65**, 23 (*nitrile, amide*)
Christian, R.V. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 1333 (*amide*)
Laing, D.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 2297 (*nitrile*)
Sargsian, M.S. *et al*, *Arm. Khim. Zh.*, 1987, **40**, 548 (*synth, pmr, ester*)
Pratt, J.A.E. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 13 (*synth, chloride, ir, pmr*)

2,4′-Oxybispyridine O-80099

2-(4-Pyridinyloxy)pyridine, 9CI. 2,4′-Dipyridyl oxide. 2,4′-Dipyridyl ether

[53258-97-2]

$C_{10}H_8N_2O$ M 172.186
Needles (pet. ether). Mp 40°.

Rockley, J.E. *et al*, *Z. Naturforsch., B*, 1982, **37**, 933 (*synth, nmr, uv, ms*)
Summers, L.A., *J. Heterocycl. Chem.*, 1987, **24**, 533 (*rev*)

3,4′-Oxybispyridine O-80100

3-(4-Pyridinyloxy)pyridine, 9CI. 3-Pyridyl 4-pyridyl ether

[53258-98-3]

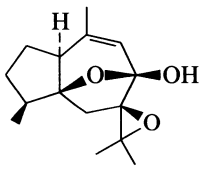
$C_{10}H_8N_2O$ M 172.186
Cryst. (hexane). Mp 48-50°.

Picrate: Cryst. Mp 145°.

Bodusek, B. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1976, **50**, 2167 (*synth, ir, pmr*)
Summers, L.A., *J. Heterocycl. Chem.*, 1987, **24**, 533 (*rev*)

Oxycurcumenol O-80101

[119205-46-8]



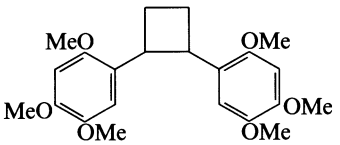
$C_{15}H_{22}O_3$ M 250.337
Constit. of *Curcuma heyneana*. Prisms (MeOH). Mp 114-116°. $[\alpha]_D^{20}$ −133° (c, 0.1 in $CHCl_3$).

Firman, K. *et al*, *Phytochemistry*, 1988, **27**, 3887.

P

Pachypophyllin **P-80001**

[114542-60-8]

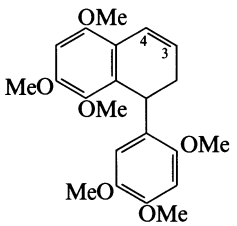


$C_{22}H_{28}O_6$ M 388.460
Constit. of *Pachypodanthium staudtii*. Cryst. (Et_2O/pet. ether). Mp 158°.

Ngadjui, B.T. *et al*, *Phytochemistry*, 1989, **28**, 231.

Pachypostaudin B **P-80002**

[114542-59-5]



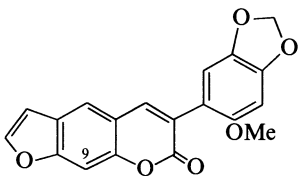
$C_{22}H_{26}O_6$ M 386.444
Constit. of *Pachypodanthium staudtii*. Needles (EtOAc/hexane). Mp 120°.

3,4-Dihydro: [114542-58-4]. ***Pachypostaudin A***
$C_{22}H_{28}O_6$ M 388.460
Constit. of *P. staudtii*. Granules (EtOAc/hexane). Mp 130°.

Ngadjui, B.T. *et al*, *Phytochemistry*, 1989, **28**, 231.

Pachyrrhizin **P-80003**

Updated Entry replacing P-00005
*6-(6-Methoxy-1,3-benzodioxol-5-yl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. 6-(2-Methoxy-4,5-methylenedioxyphenyl)furocoumarin. Neorautone*
[10091-01-7]



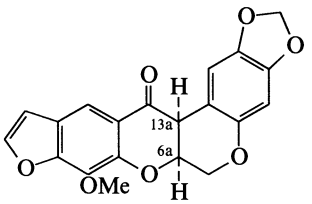
Constit. of *Pachyrrhizus erosus*, *Neoratanenia pseudopacchyrrhiza* and *N. edulis*. Yellow-green needles. Mp 207-209°.

9-Methoxy: ***Neofolin***
$C_{20}H_{14}O_7$ M 366.326
Isol. from roots of *N. ficifolia*. Greenish-yellow needles (Me_2CO, EtOAc or C_6H_6); white amorph. solid (MeOH); brownish cubes (1,2-dichloroethylene) (trimorph.). Mp 155.5-157.5° (amorph.), Mp 167-168.5° (cubes), Mp 189.5-190.5° (needles).

Norton, L.B. *et al*, *J. Am. Chem. Soc.*, 1945, **67**, 1609 (*isol*)
Simanitsch, E. *et al*, *Monatsh. Chem.*, 1957, **88**, 541 (*struct*)
Rajogopalan, P. *et al*, *Tetrahedron Lett.*, 1959, 5 (*synth*)
Abrams, C. *et al*, *CA*, 1963, **59**, 2917 (*isol*, *struct*)
Crombie, L. *et al*, *J. Chem. Soc.*, 1963, 1569 (*pmr*)
Brink, C.M. *et al*, *J. S. Afr. Chem. Inst.*, 1966, **19**, 24 (*Neofolin*)

Pachyrrhizone **P-80004**

Updated Entry replacing P-00006
*6*a,*13*a*-Dihydro-8-methoxy-1,3-dioxolo[6,7][1]benzopyrano[3,4-*b*]furo[3,2-*g*]benzopyran-13(16*H*)-one, 9CI*



$C_{20}H_{14}O_7$ M 366.326

(+)-***form*** [42485-00-7]
Constit. of the yam bean *Pachyrrhizus erosus*. Needles. Mp 232-240° dec., Mp 250-251° (sealed tube), Mp 272° (block). $[\alpha]_D^{20}$ +100° (c, 0.39 in $CHCl_3$).

Ac: Mp 147°.

Oxime: Cryst. Mp 267-268° dec. (279° block).

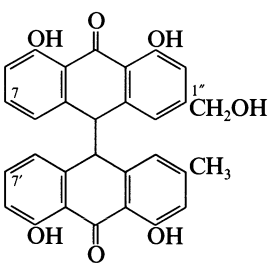
*6*a,*13*a*-Didehydro:* [28607-94-5]. ***Dehydropachyrrhizone***
$C_{20}H_{12}O_7$ M 364.311
Isol. from seeds of *P. erosus*. Pale-yellow needles ($CHCl_3$/MeOH). Mp 260-262° dec.

(±)-***form***
Mp 250° dec. (265° block).

Bickel, H. *et al*, *Helv. Chim. Acta*, 1953, **36**, 664 (*uv*, *ir*)
Krishnamurti, M. *et al*, *Tetrahedron*, 1970, **26**, 3023 (*Dehydropachyrrhizone*)
Uchiyama, M. *et al*, *Agric. Biol. Chem.*, 1973, **37**, 1227 (*synth*)

Palmidin B **P-80005**

*4,4′,5,5′-Tetrahydroxy-2-(hydroxymethyl)-2′-methyl-[9,9′-bianthracene]-10,10′(9*H*,9′*H*)-dione, 9CI. Aloeemodin-chrysophanol bianthrone*
[17062-56-5]



$C_{30}H_{22}O_7$ M 494.500
Isol. from roots of *Rheum palmatum* and fruits of *Frangula alnus*, also cascara (*Rhamnus purshiana*).

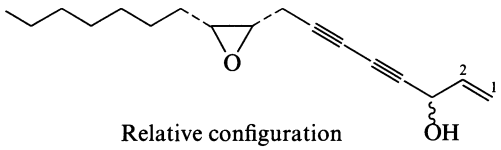
7′-Hydroxy: [17062-55-4]. ***Palmidin A.*** *Aloeemodin-emodin bianthrone*
$C_{30}H_{22}O_8$ M 510.499
From roots of *Rheum palmatum* and from cascara.

7-Hydroxy, 1″-deoxy: [17177-86-5]. ***Palmidin C.*** *Emodin-chrysophanol bianthrone*
$C_{30}H_{22}O_7$ M 494.500
From roots of *R. palmatum* and fruits of *F. alnus*, also cascara. λ_{max} 220, 272, 362 nm.

Lemli, J. *et al*, *Planta Med.*, 1964, **12**, 107.
Lemli, J., *J. Nat. Prod.* (*Lloydia*), 1965, **28**, 63 (*isol, uv*)
Kinget, R., *Planta Med.*, 6th Ed., 1967, **15**, 233 (*isol, uv*)

Panaxydol P-80006

9,10-Epoxy-1-heptadecene-4,6-diyn-3-ol. 8-(3-Heptyloxiranyl)-1-octene-4,6-diyn-3-ol, 9CI
[72800-72-7]



Relative configuration

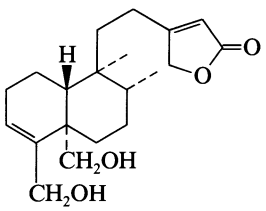
$C_{17}H_{24}O_2$ M 260.375
Isol. from *Panax ginseng*. Cytotoxic agent. $[\alpha]_D$ −19.5° (c, 0.6 in MeOH).

1,2-Dihydro, 1-chloro, 2-hydroxy: [114687-51-3]. *1-Chloro-9,10-epoxy-4,6-heptadecadiyne-2,3-diol.* ***Chloropanaxydiol***
$C_{17}H_{25}ClO_3$ M 312.835
$[\alpha]_D$ −37.2° (c, 0.2 in MeOH).

Fujimoto, Y. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4206 (*isol, pmr, cmr, struct*)

Paniculadiol P-80007

[122279-89-4]



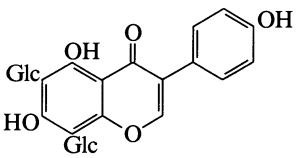
$C_{20}H_{30}O_4$ M 334.455
Constit. of *Baccharis paniculata*. Oil. $[\alpha]_D^{25}$ −1.72° (c, 0.29 in $CHCl_3$).

Di-Ac: [122297-37-4].
$C_{24}H_{34}O_6$ M 418.529
Constit. of *B. paniculata*. Oil.

Rivera, A.P. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 433 (*isol, pmr, cmr*)

Paniculatin P-80008

6,8-Di-C-glucosyl-4′,5,7-trihydroxyisoflavone. Genistein 6,8-di-C-glucoside
[32361-88-9]

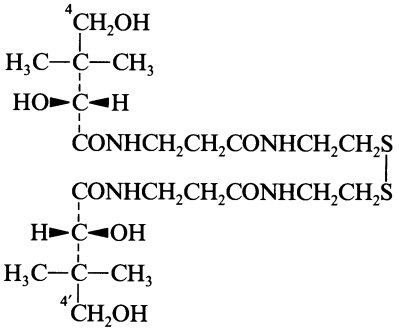


$C_{27}H_{30}O_{15}$ M 594.525
Isol. from *Dalbergia nitidula* and *D. paniculata*. Amorph. powder + $2H_2O$. Mp 225-227°.

Narayanan, V. *et al*, *Indian J. Chem.*, 1971, **9**, 14.

Pantethine P-80009

N,N′-[*Dithiobis*[*2,1-ethanediylimino*(*3-oxo-3,1-propanediyl*)]]*bis*[*2,4-dihydroxy-3,3-dimethylbutanamide*], *9CI.* N,N′-[*Dithiobis*(*ethyleneiminocarbonylethylene*)]*bis*[*2,4-dihydroxy-3,3-dimethylbutyramide*], *8CI*
[303-05-9]



$C_{22}H_{42}N_4O_8S_2$ M 554.728

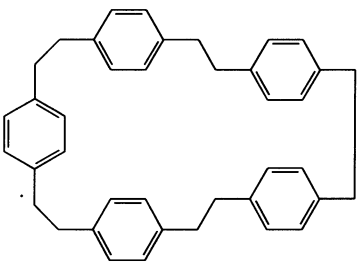
(R,R)-form [16816-67-4]
D-form
Found in foods. Bacterial growth factor. Synth. intermed. for coenzyme *A*. Cryst. (MeOH/Me_2CO), glass (H_2O). $[\alpha]_D^{22}$ +17.9° (c,3.2 in H_2O). Hydrol. by acids.

4,4′-Diphosphate: [17451-69-3].
$C_{22}H_{40}N_4O_{14}P_2S_2$ M 710.656
Intermediate for coenzyme *A* synthesis. Powder (MeOH)(as Ba salt). $[\alpha]_D^{20}$ +12.2° (c, 1 in H_2O).

Brown, G.M. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 1691 (*occur, purifn*)
Viscontini, M. *et al*, *Helv. Chim. Acta*, 1954, **37**, 375 (*synth, tlc, deriv*)
Bowman, R.E. *et al*, *J. Chem. Soc.*, 1954, 1171 (*anal, rev, bibl*)
Moffatt, J.G. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 663 (*chromatog*)
Shimizu, M. *et al*, *Chem. Pharm. Bull.*, 1965, **13**, 180 (*synth, chromatog, ir, uv*)
Nagase, O., *Chem. Pharm. Bull.*, 1967, **15**, 648 (*phosphate, synth*)
Zhdanovich, E.S. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1967, **37**, 337 (*synth, ir*)
Hashimoto, M. *et al*, *Chem. Lett.*, 1972, 595 (*synth*)

[2.2.2.2.2]Paracyclophane P-80010

Hexacyclo[*26.2.2.2*^{4,7}.*2*^{10,13}.*2*^{16,19}.*2*^{22,25}]*tetraconta-4,6,10,12,16,18,22,24,28,30,31,33,35,37,39-pentadecaene, 9CI*
[43082-13-9]



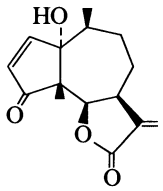
$C_{40}H_{40}$ M 520.756
Mp 172°.

Schmidbaur, H. *et al*, *Chem. Ber.*, 1988, **121**, 1341 (*synth, ir, ms, cryst struct*)

Parthenin P-80011

Updated Entry replacing P-30015

[508-59-8]



$C_{15}H_{18}O_4$ M 262.305

Bitter principle of *Parthenium hysterophorum* and *Iva nevadensis*. Cryst. (H_2O). Mp 163-166°. $[\alpha]_D^{25}$ +7.02° (c, 2.71 in $CHCl_3$).

▷ BD9635000.

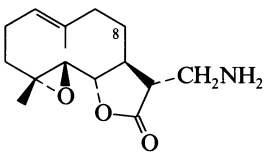
11,13-Dihydro: ***Dihydroparthenin***

$C_{15}H_{20}O_4$ M 264.321

Constit. of *P. hysterophorus*. Cryst. Mp 145°.

Herz, W. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 2601 (*isol, struct*)
Kok, P. *et al*, *Bull. Soc. Chim. Belg.*, 1978, **87**, 615 (*synth*)
Heathcock, C.H. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 6081 (*synth*)
Talwar, K.K. *et al*, *Phytochemistry*, 1989, **28**, 1091 (*deriv*)

Parthenolidine P-80012



$C_{15}H_{23}NO_3$ M 265.352

N-*Ac:* [119766-96-0]. **N-*Acetylparthenolidine***

$C_{17}H_{25}NO_4$ M 307.389

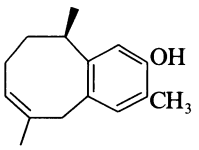
Constit. of *Michelia rajaniana* (Magnoliaceae). Oil. $[\alpha]_D^{24}$ +23° (c, 0.67 in $CHCl_3$).

Ruangrungsi, N. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1220 (*isol, pmr, cmr*)

Parvifoline P-80013

Updated Entry replacing P-10011

[62706-41-6]



$C_{15}H_{20}O$ M 216.322

Constit. of *Coreopsis parvifolia* and *Perezia carpholepis*. Needles (Me_2CO/hexane). Mp 85-86°. $[\alpha]_D$ −173° (c, 1.73 in $CHCl_3$).

Ac:

$C_{17}H_{22}O_2$ M 258.360

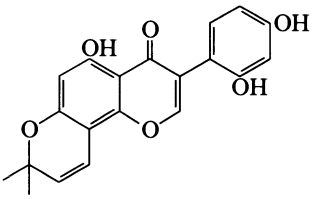
Cryst. (Me_2CO/hexane). Mp 59-61°. $[\alpha]_D$ −98° ($CHCl_3$).

Bohlmann, F. *et al*, *Chem. Ber.*, 1977, **110**, 468 (*struct*)
Joseph-Naphan, P. *et al*, *Phytochemistry*, 1982, **21**, 669 (*struct*)
Joseph-Naphan, P. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 675 (*abs config*)

Parvisoflavone A P-80014

*3-(2,4-Dihydroxyphenyl)-5-hydroxy-8,8-dimethyl-4*H, *8*H-*benzo[1,2-*b*:3,4-*b′*]dipyran-4-one, 9CI*

[50277-01-5]



$C_{20}H_{16}O_6$ M 352.343

Obt. only as a mixt. with Parvisoflavone B, P-80015. Isol. from trunkwood of *Poecilanthe parviflora*. Yellow cryst. ($Me_2CO/CHCl_3$) (mixt.). Mp 235-239°.

Tri-Me ether: Mp 166-168°. Pure.

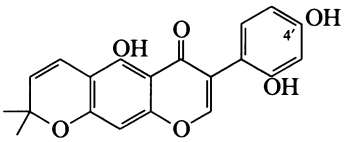
Assumpção, R.M.V. *et al*, *Phytochemistry*, 1973, **12**, 1188 (*isol, uv, ir, pmr, ms, struct*)

Parvisoflavone B P-80015

Updated Entry replacing I-00887

*7-(2,4-Dihydroxyphenyl)-5-hydroxy-2,2-dimethyl-2*H,*6*H-*benzo[1,2-*b*:5,4-*b′*]dipyran-6-one, 9CI*

[50277-02-6]



$C_{20}H_{16}O_6$ M 352.343

Obt. only as a mixt. with Parvisoflavone A, P-80014. Isol. from trunkwood of *Poecilanthe parviflora*.

Tri-Me ether: Cryst. Mp 149-151°. This deriv. obt. in pure state.

4′-O-(3-Methyl-2-butenyl): [30431-67-5]. ***Isoauriculatin***

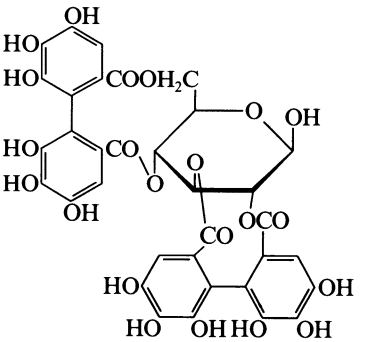
$C_{25}H_{24}O_6$ M 420.461

Constit. of *Milletia auriculata*. Pale-yellow plates. Mp 132-134°.

Assumpção, R.M.V. *et al*, *Phytochemistry*, 1973, **12**, 1188 (*isol, uv, ir, pmr, ms, struct*)
Minhaj, T.V. *et al*, *Tetrahedron*, 1976, **32**, 749 (*Isoauriculatin*)

Pedunculagin P-80016

[7045-42-3]

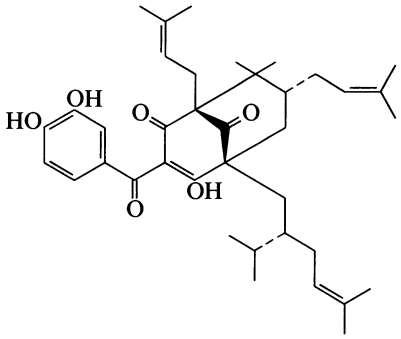


$C_{34}H_{24}O_{22}$ M 784.550

Isol. from *Quercus robor* and *Q. sessiliflora*. Amorph. sandy solid. $[\alpha]_D^{25}$ +106° (c, 2 in MeOH).

Schmidt, O.T. *et al*, *Justus Liebigs Ann. Chem.*, 1965, **690**, 150.

Pedunculol P-80017



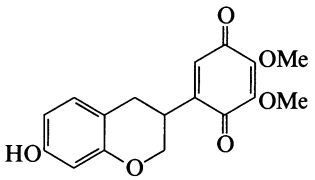
$C_{38}H_{52}O_6$ M 604.825
Constit. of *Garcinia pedunculata*. Yellow cryst. (C_6H_6). Mp 125°. $[\alpha]_D^{25}$ −159° (EtOH).

Sahu, A. *et al*, *Phytochemistry*, 1989, **28**, 1239.

Pendulone P-80018

*5-(3,4-Dihydro-7-hydroxy-2*H*-1-benzopyran-3-yl)-2,3-dimethoxy-2,5-cyclohexadiene-1,4-dione, 9CI. 7-Hydroxy-3′,4′-dimethoxyisoflavanquinone*

[69359-09-7]



$C_{17}H_{16}O_6$ M 316.310
Tentative struct. Isol. from heartwood of *Millettia pendula*.

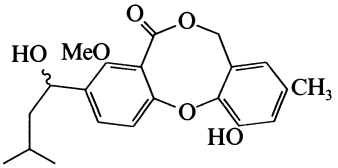
Hayashi, Y. *et al*, *Mokuzai Gakkaishi*, 1978, **24**, 898; *CA*, **90**, 100111p.

Penicillide P-80019

Updated Entry replacing P-00207

*11-Hydroxy-3-(1-hydroxy-3-methylbutyl)-4-methoxy-9-methyl-5*H*,7*H*-dibenzo*[b,g][*1,5*]*dioxocin-5-one, 9CI*

[55303-92-9]



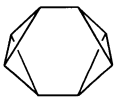
$C_{21}H_{24}O_6$ M 372.417
Metab. of *Penicillium* spp. Plant growth inhibitor.
Me ether: Mp 128-129.5°. $[\alpha]_D^{27}$ +14.4° (MeOH).

Sassa, T. *et al*, *Tetrahedron Lett.*, 1974, 3941 (*isol, struct, uv, ms*)

Pentacyclo[5.1.0.0^{2,4}.0^{3,5}.0^{6,8}]octane P-80020

Octabisvalene

[35434-67-4]



C_8H_8 M 104.151
Solid. Mp 27-30°.

Rücker, C. *et al*, *Chem. Ber.*, 1987, **120**, 1629.
Rücker, C. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4828 (*synth, ms, ir, pmr, cmr*)

6,8,10,12-Pentadecatetraenal, 9CI P-80021

[13894-86-5]

$H_3CCH_2CH{=}CHCH{=}CHCH{=}CHCH{=}CH(CH_2)_4CHO$

$C_{15}H_{22}O$ M 218.338
Isol. from leaves of *Centaurea* spp. Cryst. Mp <20°. An (*E,E,E,Z*)-form with exact config. unknown.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3544 (*isol, uv, pmr*)
Andersen, A.B. *et al*, *Phytochemistry*, 1977, **16**, 1829 (*isol*)

1,8,10,14-Pentadecatetraene-4,6-diyn-3-ol P-80022

$H_2C{=}CHCH_2CH_2CH{=}CHCH{=}CHC{\equiv}CC{\equiv}CCH(OH)CH{=}CH_2$

$C_{15}H_{16}O$ M 212.291
(E,E)-form [17486-46-3]
Isol. from *Cotula coronopifolia*. Oil. λ_{max} 226, 236, 294, 309 nm. Not obt. pure.
p-*Phenylazobenzoyl:* Cryst. (pet. ether). Mp 44.5-46°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2828; 1967, **100**, 3450 (*isol, struct, synth*)

8,10,14-Pentadecatriene-4,6-diyn-3-ol P-80023

$H_2C{=}CHCH_2CH_2CH{=}CHCH{=}CHC{\equiv}CC{\equiv}CCH(OH)CH_2CH_3$

$C_{15}H_{18}O$ M 214.307
(E,E)-form [13028-53-0]
Isol. from above-ground parts of *Cotula coronopifolia*. Oil. λ_{max} 226, 236, 294, 309 nm (Et_2O). Not obt. pure.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2828; 1967, **100**, 3450 (*isol, struct, synth*)

10-Pentadecenal P-80024

[60671-80-9]

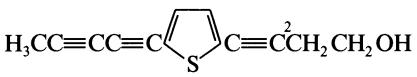
$H_3C(CH_2)_3CH{=}CH(CH_2)_8CHO$

$C_{15}H_{28}O$ M 224.386

Kubo, I. *et al*, *Tetrahedron*, 1987, **43**, 2653 (*synth, ir, pmr*)

4-[5-(1,3-Pentadiynyl)-7-thienyl]-3-butyn-1-ol, 9CI P-80025

[1209-21-8]



$C_{13}H_{10}OS$ M 214.287
Isol. from oil of *Echinops sphaerocephalus*. Oil. λ_{max} 319, 339 nm.
p-*Phenylazobenzoyl:* [26968-51-4].
Cryst. (Et_2O/pet. ether). Mp 126°.
Ac: 1-Acetoxy-4-[5-(1,3-pentadiynyl)-2-thienyl]-3-butyne
$C_{15}H_{12}O_2S$ M 256.325
Isol. from *E. sphaerocephalus*. Oil. λ_{max}232, 245, 319, 339 nm.
2-Hydroxy: [1212-60-8]. *4-[5-(1,3-Pentadiynyl)-2-thienyl]-3-butyne-1,2-diol, 9CI*
$C_{13}H_{10}O_2S$ M 230.287

Isol. from *E. sphaerocephalus* and other plants. Cryst. (CCl_4). Mp 112°.

2-Hydroxy, 1-Ac: [26905-72-6].
$C_{15}H_{12}O_3S$ M 272.324
Isol. from *Eclipta erecta*. Yellowish oil. λ_{max} 340, 320 nm.

2-Hydroxy, 2-Ac:
$C_{15}H_{12}O_3S$ M 272.324
Isol. from *Pluchea suaveolens*.

2-Hydroxy, di-Ac: [1161-52-0]. *2-(1,3-Pentadiynyl)-5-(3,4-diacetoxy-1-butynyl)thiophene*
$C_{17}H_{14}O_4S$ M 314.361
Isol. from *E. sphaerocephalus*. Oil.

2-Chloro: [1142-35-4]. ***2-Chloro-4-[5-(1,3-pentadiynyl)-2-thienyl]-3-butyn-1-ol*, 9CI**
$C_{13}H_9ClOS$ M 248.732
Isol. from *E. sphaerocephalus* and *Pluchea* sp. Oil.

2-Chloro, Ac: [1152-72-3]. *2-(3-Chloro-4-acetoxy-1-butynyl)-5-(1,3-pentadiynyl)thiophene*
$C_{15}H_{11}ClO_2S$ M 290.769
Isol. from *E. sphaerocephalus* and from roots of *Centaurea cristata*. Oil. λ_{max} 207.5, 233, 245, 320, 340.5 nm.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 155, 876 (*isol, uv, ir, pmr, struct, biosynth*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3544; 1968, **101**, 4163; 1970, **103**, 834 (*isol, synth, derivs*)
Bohlmann, F. *et al*, *Phytochemistry*, 1980, **19**, 969 (*deriv*)
Dawidar, A. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 5068 (*deriv*)

Pentafluoronitrobenzene, 9CI — P-80026

[880-78-4]

$(C_6F_5)NO_2$

$C_6F_5NO_2$ M 213.063
Golden yellow liq. Bp 158-161°, Bp_{52} 91-94°. Lachrymator.

Brooke, G.M. *et al*, *J. Chem. Soc.*, 1961, 802 (*synth*)
Bruce, M.I., *J. Chem. Soc. A*, 1968, 1459 (*F nmr*)
Briggs, J.M. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1973, 1789 (*cmr*)
Trudell, B.G. *et al*, *Can. J. Chem.*, 1978, **56**, 538 (*pe*)
Funn, G.G. *et al*, *J. Fluorine Chem.*, 1985, **28**, 241 (*cryst struct*)
Korobeinicheva, I.K. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1987, 1766 (*raman*)

Pentafluorophenylacetic acid — P-80027

2,3,4,5,6-Pentafluorobenzeneacetic acid, 9CI

[653-21-4]

$(C_6F_5)CH_2COOH$

$C_8H_3F_5O_2$ M 226.102
Cryst. (pet. ether). Mp 109°.

Et ester: [784-35-0].
$C_{10}H_7F_5O_2$ M 254.156
Bp_{14} 94-96°.

Chloride: [832-72-4].
$C_8H_2ClF_5O$ M 244.548
Bp_{29} 90-95°.

Amide:
$C_8H_4F_5NO$ M 225.118
Cryst. ($EtOH/C_6H_6$). Mp 187-188°.

Nitrile: [653-30-5]. *Pentafluorophenylacetonitrile. (Cyanomethyl)pentafluorobenzene*
$C_8H_2F_5N$ M 207.102
Mp 38-38.5°. Bp_8 105°.

Barbour, A.K. *et al*, *J. Chem. Soc.*, 1961, 808 (*synth, ir*)
Org. Synth., 1977, **57**, 80 (*nitrile*)
Bordwell, F.G. *et al*, *J. Org. Chem.*, 1988, **53**, 780 (*nitrile*)

1,1,3,3,3-Pentafluoro-1-propene, 9CI — P-80028

2H-Pentafluoropropylene

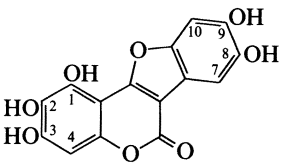
[690-27-7]

$F_3CCH{=}CF_2$

C_3HF_5 M 132.033
Mp −160.9°. Bp −21° (−17°, −29°).

Banks, R.E. *et al*, *Proc. Chem. Soc., London*, 1964, 121 (*synth*)
Sianesi, D. *et al*, *Ann. Chim. (Rome)*, 1965, **55**, 872 (*synth, ir*)

1,2,3,8,9-Pentahydroxycoumestan — P-80029

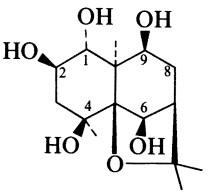


$C_{15}H_8O_8$ M 316.223

1,3-Di-Me, 8,9-methylene ether: [35930-41-7]. ***2-Hydroxy-1,3-dimethoxy-8,9-methylenedioxycoumestan***
$C_{18}H_{12}O_8$ M 356.288
Isol. from heartwood of *Swartzia leiocalycina*.

Donnelly, D.M.X. *et al*, *Phytochemistry*, 1971, **10**, 3147.

1,2,4,6,9-Pentahydroxydihydro-β-agarofuran — P-80030



$C_{15}H_{26}O_6$ M 302.367

(1α,2β,6β,9β)-form

1-Cinnamoyl, 6-(3-pyridinecarbonyl), 9-Ac: ***9β-Acetoxy-1α-cinnamoyloxy-2β,4β-dihydroxy-6β-nicotinoyloxydihydro-β-agarofuran.*** *1α-Cinnamoyloxy-6β-nicotinoyloxy-9β-acetoxy-2β,4β-dihydroxydihydro-β-agarofuran*
$C_{30}H_{33}NO_7$ M 519.593
Alkaloid from the aerial parts of *Orthosphaenia mexicana* (Celastraceae). Amorph. solid.

6,9-Di-Ac, 1-cinnamoyl: ***6β,9β-Diacetoxy-1α-cinnamoyloxy-2β,4β-hydroxydihydro-β-agarofuran***
$C_{28}H_{36}O_9$ M 516.587
Constit. of *Orthosphenia mexicana*.

González, A.G. *et al*, *Phytochemistry*, 1987, **26**, 2133; 1988, **27**, 473 (*isol, ir, pmr, ms, struct*)

1,4,6,8,9-Pentahydroxydihydro-β-agarofuran — P-80031

$C_{15}H_{26}O_6$ M 302.367

(1α,6β,8β,9α)-form

1-Benzoyl, 6-(3-pyridinecarbonyl), 9-Ac: ***9α-Acetoxy-1α-benzoyloxy-4β,8β-dihydroxy-6β-nicotinoyloxydihydro-β-agarofuran.*** *1α-Benzoyloxy-6β-nicotinoyloxy-9α-acetoxy-4β,8β-dihydroxydihydro-β-agarofuran*
$C_{30}H_{35}NO_9$ M 553.608
Alkaloid from the aerial parts of *Orthosphaenia mexicana* (Celastraceae). Mp 184-186°.

1-Benzoyl, 6-(3-pyridinecarbonyl), 8,9-Di-Ac: ***8β,9α-Diacetoxy-1α-benzoyloxy-4β-hydroxy-6β-nicotinoyl-β-agarofuran.***

nicotinoyloxy-8β,9α-diacetoxy-4β-hydroxydihydro-β-agarofuran
$C_{32}H_{37}NO_{10}$ M 595.645
Alkaloid from the root bark of *Rzedowskia tolantonguensis* (Celastraceae). Mp 114-116°. *Rzedowskia* is not a generally recognised genus.

6,9-Di-Ac, 1-benzoyl: 6β,9α-Diacetoxy-1α-benzoyloxy-4β,8β-dihydroxydihydro-β-agarofuran
$C_{26}H_{34}O_9$ M 490.549
Constit. of *Orthosphenia mexicana*. Cryst. Mp 194-198°.

6,8,9-Tri-Ac, 1-benzoyl: 6β,8β,9α-Triacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran
$C_{28}H_{36}O_{10}$ M 532.586
Constit. of *O. mexicana*. Cryst. Mp 76-80°.

(1α,6β,8β,9β)-form

1-Benzoyl, 6β-(3-pyridinecarbonyl), 9-Ac: ***9β-Acetoxy-1α-benzoyloxy-4β-hydroxy-6β-nicotinoyloxydihydro-β-agarofuran.*** *1α-Benzoyloxy-6β-nicotinoyloxy-9β-acetoxy-4β-hydroxydihydro-β-agarofuran*
$C_{30}H_{35}NO_8$ M 537.608
Alkaloid from the aerial parts of *O. mexicana* and the root bark of *R. tolantonguensis* (Celastraceae). Mp 139-148°.

González, A.G. *et al*, *Phytochemistry*, 1987, **26**, 2133; 1988, **27**, 473 (*isol, ir, uv, pmr, ms, struct*)

1,4,6,9,15-Pentahydroxydihydro-β-agarofuran P-80032

$C_{15}H_{26}O_6$ M 302.367

(1α,4β,6β,9β)-form

6,9,15-Tri-Ac, 1-benzoyl: 6β,9β,15-Triacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran
$C_{28}H_{36}O_{10}$ M 532.586
Constit. of *Orthosphenia mexicana*. Cryst. Mp 188-190°.

González, A.G. *et al*, *Phytochemistry*, 1988, **27**, 473.

2′,4′,5,5′,7-Pentahydroxyflavone P-80033

$C_{15}H_{10}O_7$ M 302.240

4′,5′-Di-Me ether: 2′,5,7-Trihydroxy-4′,5′-dimethoxyflavone. 2′-Hydoxy-5′-methoxybiochanin A
$C_{17}H_{14}O_7$ M 330.293
Constit. of *Erythrina eriotriocha*. Needles ($MeOH/CH_2Cl_2$). Mp 250°.

Nkengfack, A.E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 320 (*isol, pmr, cmr*)

2′,4′,5,7,8-Pentahydroxyflavone P-80034

$C_{15}H_{10}O_7$ M 302.240

2′,4′,7,8-Tetra-Me ether: 5-Hydroxy-2′,4′,7,8-tetramethoxyflavone
$C_{19}H_{18}O_7$ M 358.347
Constit. of *Limnophila rugosa*. Cryst. Mp 188-189°.

Mukherjee, K.S. *et al*, *Phytochemistry*, 1989, **28**, 1778.

3,4′,5,6,7-Pentahydroxyflavone P-80035

Updated Entry replacing P-60047

[4324-55-4]

$C_{15}H_{10}O_7$ M 302.240
Yellow cryst. ($EtOH/Me_2CO$). Mp 328-330°.

5,6-Di-Me ether: 3,4′,7-Trihydroxy-5,6-dimethoxyflavone
$C_{17}H_{14}O_7$ M 330.293
Constit. of *Adenostoma sparsifolium*.

6,7-Di-Me ether: [29536-41-2]. *3,4′,5-Trihydroxy-6,7-dimethoxyflavone.* ***Eupalitin***
$C_{17}H_{14}O_7$ M 330.293
Constit. of *Eupatorium* spp. Cryst. Mp 291-292°.

6,7-Di-Me ether, O^3-rhamnoside: [29617-75-2]. ***Eupalin***
$C_{23}H_{24}O_{11}$ M 476.436
Constit. of the aerial parts of *Eupatorium ligustrinum* and of *Rudbeckia bicolor*. Cryst. (MeOH). Mp 207-210° (189°). $[\alpha]_D$ −129.6° (Py).

3,6,7-Tri-Me ether: [569-80-2]. *4′,5-Dihydroxy-3,6,7-trimethoxyflavone.* ***Penduletin***
$C_{18}H_{16}O_7$ M 344.320
Constit. of *Tephrosia candida*. Yellow cryst. (MeOH). Mp 222°.

4′,6,7-Tri-Me ether: [4324-53-2]. *3,5-Dihydroxy-4′,6,7-trimethoxyflavone.* ***Mikanin***
$C_{18}H_{16}O_7$ M 344.320
Constit. of *Mikania cordata*. Bright-yellow cryst. (C_6H_6 or $CHCl_3/MeOH$). Mp 222-224°.

5,6,7-Tri-Me ether: [35286-55-6]. *3,4′-Dihydroxy-5,6,7-trimethoxyflavone.* ***Candidol***
$C_{18}H_{16}O_7$ M 344.320
Constit. of *Tephrosia candida*. Cryst. Mp 253-254°.

3,4′,6-Tri-Me ether: [27782-63-4]. *5,7-Dihydroxy-3,4′-6-trimethoxyflavone.* ***Santin***
$C_{18}H_{16}O_7$ M 344.320
Isol. from *Chrysanthemum parthenium*. Cryst. (C_6H_6/EtOAc). Mp 164-165°.

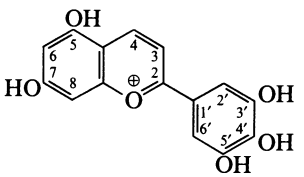
3,4′,6,7-Tetra-Me ether: [14787-34-9]. *5-Hydroxy-3,4′,6,7-tetramethoxyflavone*
$C_{19}H_{18}O_7$ M 358.347
Constit. of *Blumea malcomii, Dodonaea lobulata* and *D. viscosa*. Cryst. Mp 178-180° (151.5-153°).

Penta-Me ether: [4472-73-5]. *3,4′,5,6,7-Pentamethoxyflavone*
$C_{20}H_{20}O_7$ M 372.374
Needles. Mp 157-158° (151-153°).

Kiang, A.K. *et al*, *J. Chem. Soc.*, 1965, 6371 (*synth*)
Wagner, H. *et al*, *Tetrahedron Lett.*, 1965, 3849 (*synth*)
Dawson, R.M. *et al*, *Aust. J. Chem.*, 1966, **19**, 2133 (*isol*)
Wagner, H. *et al*, *Chem. Ber.*, 1967, **100**, 1768 (*synth*)
Sim, K.Y., *J. Chem. Soc. C*, 1967, 976 (*synth*)
Quijano, L. *et al*, *Tetrahedron*, 1970, **26**, 2851 (*Eupalin*)
Southwick, L. *et al*, *Phytochemistry*, 1972, **11**, 2351 (*isol, struct*)
Rodriguez, E. *et al*, *Phytochemistry*, 1972, **11**, 3509 (*isol, struct*)
Wagner, H. *et al*, *Chem. Ber.*, 1974, **107**, 1049 (*synth*)
Jauhari, P.K. *et al*, *Phytochemistry*, 1979, **18**, 359 (*isol*)
Proksch, M. *et al*, *Phytochemistry*, 1982, **21**, 2893 (*isol*)
Sachdev, K. *et al*, *Phytochemistry*, 1983, **22**, 1253 (*isol*)
Dutt, S.K. *et al*, *Phytochemistry*, 1983, **22**, 325 (*isol*)
Kulkarni, M.M. *et al*, *Phytochemistry*, 1987, **26**, 2079 (*isol*)
Parmar, V.S. *et al*, *Tetrahedron*, 1987, **43**, 4241 (*cryst struct*)
Horie, T. *et al*, *Phytochemistry*, 1988, **27**, 1491 (*synth, struct*)
Markham, K.R., *Phytochemistry*, 1989, **28**, 243 (*struct*)

3′,4′,5,5′,7-Pentahydroxyflavylium P-80036

Tricetinidin



$C_{15}H_{11}O_6^{\oplus}$ M 287.248
Isol. from black tea (*Thea sinensis*) and prob. as glycoside from *Dryopteris erythrosora*.

Chloride:
$C_{15}H_{11}ClO_6$ M 322.701

λ_{max} 281, 513 nm (MOH + HCl); λ_{max} 564 nm (MeOH + NaOH).

Roberts, E.A.H. *et al*, *J. Sci. Food Agric.*, 1957, **8**, 72; 1958, **9**, 217.

Harborne, J.B., *Phytochemistry*, 1966, **5**, 589.

3′,4′,5,7,8-Pentahydroxyflavylium P-80037

Columnidin

$C_{15}H_{11}O_6^{\oplus}$ M 287.248

Chloride:

$C_{15}H_{11}ClO_6$ M 322.701

λ_{max} 275, 511 nm (MeOH + HCl); λ_{max} 560 nm (MeOH + NaOH).

O-*Glucoside:* ***Columnin***

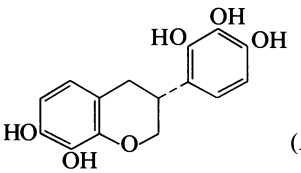
$C_{21}H_{21}O_{11}^{\oplus}$ M 449.390

Isol. from *Columnea banksii*. Dark-red cryst. (EtOH) (as chloride).

Harborne, J.B., *Phytochemistry*, 1966, **5**, 589.

2′,3′,4′,7,8-Pentahydroxyisoflavan P-80038

Updated Entry replacing D-05095



(*R*)-*form*

$C_{15}H_{14}O_6$ M 290.272

(R)-form

2′,4′-Di-Me ether: [50439-57-1]. *3′,7,8-Trihydroxy-2′,4′-dimethoxyisoflavan. 8-Demethylduartin*

$C_{17}H_{18}O_6$ M 318.326

Isol. from wood of *Dalbergia ecastophyllum*.

2′,4′-Di-Me ether, tri-Ac: Needles (MeOH). Mp 223.5-225°. $[\alpha]_D^{22}$ +22.3° ($CHCl_3$).

(S)-form

2′,4′,8-Tri-Me ether: [52305-04-1]. *3′,7-Dihydroxy-2′,4′,8-trimethoxyisoflavan.* ***Duartin***

$C_{18}H_{20}O_6$ M 332.352

Constit. of the wood of *Machaerium acutifolium*, *M. mucronulatum*, *M. opacum* and *M. villosium*. Needles (MeOH). Mp 145°. $[\alpha]_D$ −25° (Me_2CO), $[\alpha]_D^{20}$ −18.5° (c, 1.68 in $CHCl_3$).

2′,4′,8-Tri-Me ether, di-Ac: Cryst. (EtOH). Mp 101°. $[\alpha]_D^{20}$ −22° (c, 2.08 in $CHCl_3$).

(±)-form

2′,4′-Di-Me ether, tri-Ac: Mp 236-237°.

2′,4′,8-Tri-Me ether: Prisms (EtOH). Mp 199-201° (195°).

Kurosawa, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 1263, 1265 (*Duartin*)

Donnelly, D.M.X. *et al*, *Phytochemistry*, 1973, **12**, 1157 (8-*Demethylduartin*)

Farkas, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1974, 305 (*synth*)

Wenkert, E. *et al*, *Phytochemistry*, 1977, **16**, 1811 (*cmr*)

Ollis, D.W. *et al*, *Phytochemistry*, 1978, **17**, 1401 (*isol, synth*)

Kurosawa, K. *et al*, *Phytochemistry*, 1978, **17**, 1423 (*isol, abs config*)

2′,3′,4′,5,7-Pentahydroxyisoflavanone P-80039

*2,3-Dihydro-5,7-dihydroxy-3-(2,3,4-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{12}O_7$ M 304.256

2′,3′-Di-Me ether: [49776-79-6]. *4′,5,7-Trihydroxy-2′,3′-dimethoxyisoflavanone.* ***Parvisoflavanone***

$C_{17}H_{16}O_7$ M 332.309

Isol. from trunkwood of *Poecilanthe parviflora*. Prisms (MeOH). Mp 203-205°. Incorr. referred to also as Parvisoflavone.

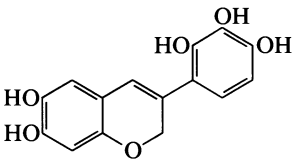
Penta-Me ether: [49776-80-9]. *2′,3′,4′,5,7-Pentamethoxyisoflavanone*

$C_{20}H_{22}O_7$ M 374.390

Needles (MeOH). Mp 159-162°. Incorr. referred to as Di-*O*-methylparvisoflavone.

Assumpcão, R.M.V. *et al*, *Phytochemistry*, 1973, **12**, 1188.

2′,3′,4′,6,7-Pentahydroxyisoflavene P-80040



$C_{15}H_{12}O_6$ M 288.256

2′,4′ or 3′,4′-Di-Me ether: [78900-89-7].

$C_{17}H_{16}O_6$ M 316.310

Isol. from *Baphia nitida* heartwood.

Di-Me ether, tri-Ac: Mp 52-55°.

Arnone, A. *et al*, *Phytochemistry*, 1981, **20**, 799 (*isol, pmr*)

2′,4′,5,5′,7-Pentahydroxyisoflavone P-80041

*5,7-Dihydroxy-3-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{10}O_7$ M 302.240

2′,5′,7-Tri-Me ether: [73428-16-7]. *4′,5-Dihydroxy-2′,5′,7-trimethoxyisoflavone.* ***Derrugenin***

$C_{18}H_{16}O_7$ M 344.320

Isol. from seed hulls of *Derris robusta*. Mp 218-219°. Revised struct.

2′,4′,5′,7-Tetra-Me ether: [72545-39-2]. *5-Hydroxy-2′,4′,5′,7-tetramethoxyisoflavone.* ***Robustigenin***

$C_{19}H_{18}O_7$ M 358.347

Isol. from *D. robusta* seed hulls. Cryst.

2′,4′,5′,7-Tetra-Me ether, Ac: Needles. Mp 168°.

Penta-Me ether: [72545-41-6]. *2′,4′,5,5′,7-Pentamethoxyisoflavone. Robustigenin methyl ether*

$C_{20}H_{20}O_7$ M 372.374

Isol. from *D. robusta* seed hulls. Needles. Mp 192-193°.

Chibber, S.S. *et al*, *Indian J. Chem., Sect. B*, 1979, **17**, 649 (*Robustigenin methyl ether*)

Chibber, S.S. *et al*, *Phytochemistry*, 1979, **18**, 1082, 1583 (*Robustigenin, Derrugenin*)

2′,4′,5′,6,7-Pentahydroxyisoflavone P-80042

*6,7-Dihydroxy-3-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{10}O_7$ M 302.240

2′,6-Di-Me, 4′,5′-methylenedioxy ether: [40009-88-9]. *7-Hydroxy-2′,6-dimethoxy-3′,4′-methylenedioxyisoflavone.* ***Dalpatein***

$C_{18}H_{14}O_7$ M 342.304

Isol. from seeds of *Dalbergia paniculata*. Needles ($CHCl_3$/MeOH). Mp 253-254°.

2′,6-Di-Me, 4′,5′-methylenedioxy ether, 7-O-β-D-glucopyranoside: see 7-O-β-D-Glucopyranoside [40522-40-5]. ***Dalpatin***

$C_{24}H_{24}O_{12}$ M 504.446

Isol. from *D. paniculata*. Needles (EtOH). Mp 261-263° dec.

2′,7-Di-Me, 4′,5′-methylenedioxy ether: [51986-37-9]. *6-Hydroxy-2′,7-dimethoxy-4′,5′-methylenedioxyisoflavone*
$C_{18}H_{14}O_7$ M 342.304
Isol. from *Cordyla africana, Dalbergia assamica* and *Mildbraedeodendron excelsa*. Needles (MeOH). Mp 252-253°.

2′,6,7-Tri-Me, 4′,5′-methylenedioxy ether: [24195-15-1]. *2′,6,7-Trimethoxy-4′,5′-methylenedioxyisoflavone.* ***Milldurone***
$C_{19}H_{16}O_7$ M 356.331
Isol. from *C. africana, D. paniculata, M. excelsa, Millettia dura, Pterodon apparicioi* and *P. pubescens*. Fine cryst. (MeOH). Mp 233-234°.

2′,4′,5′,6-Tetra-Me ether: [22773-72-4]. *7-Hydroxy-2′,4′,5′,6-tetramethoxyisoflavone*
$C_{19}H_{18}O_7$ M 358.347
Isol. from *P. apparicioi* trunkwood. Needles. Mp 205-207°.

Penta-Me ether: [24203-68-7]. *2′,4′,5′,6,7-Pentamethoxyisoflavone*
$C_{20}H_{20}O_7$ M 372.374
Isol. from *C. africana, Mildbraeodendron excelsa, P. apparicioi* and *P. pubescens*. Needles (MeOH). Mp 171-172°.

Ollis, W.D. *et al, Tetrahedron*, 1967, **23**, 4741 (*Milldurone*)
Campbell, R.V.M. *et al, J. Chem. Soc. C*, 1969, 1787 (*isol*)
Nógrádi, M. *et al, Chem. Ber.*, 1970, **103**, 999 (*synth*)
Adinarayana, D. *et al, Tetrahedron*, 1972, **28**, 5377 (*Dalpatin*)
Campbell, R.V.M. *et al, J. Chem. Soc., Perkin Trans.* 1, 1973, 2222 (*6-hydroxy-2′,7-dimethoxy-4′,5′-methylenedioxyisoflavone*)
Galina, E. *et al, Phytochemistry*, 1974, **13**, 2593 (*isol*)
Meegan, M.J. *et al, Phytochemistry*, 1975, **14**, 2283 (*isol*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

3′,4′,5,6,7-Pentahydroxyisoflavone P-80043

Updated Entry replacing T-03329

*3-(3,4-Dihydroxyphenyl)-5,6,7-trihydroxy-4*H*-1-benzopyran-4-one, 9CI*
$C_{15}H_{10}O_6$ M 286.240

3′,6-Di-Me ether: [39012-01-6]. *4′,5,7-Trihydroxy-3′,6-dimethoxyisoflavone.* ***Iristectorigenin B***
$C_{17}H_{14}O_7$ M 330.293
Isol. from rhizomes of *I. florentina* and *I. germanica*. Pale-yellow needles (MeOH). Mp 153°.

3′,6-Di-Me ether, glucoside: ***Iristectorin B***
$C_{23}H_{24}O_{12}$ M 492.435
Isol. from rhizomes of *I. tectorum*. Posn. of glycosyl residue not sure.

4′,6-Di-Me ether: [37744-62-0]. *3′,5,7-Trihydoxy-4′,6-dimethoxyisoflavone.* ***Iristectorigenin A***
$C_{17}H_{14}O_7$ M 330.293
Isol. from *Iris germanica, I. unguicularis, Monopteryx inpae* and from cultures of *Streptomyces* sp. Shows antihypertensive props. Mp 231°. All isolations of isoflavones from microorganisms are considered suspect.

4′,6-Di-Me ether, 7-O-β-D-glucopyranoside: [37744-61-9]. ***Iristectorin A***
$C_{23}H_{24}O_{12}$ M 492.435
Constit. of *I. tectorum*. Mp 212-214°.

3′,4′,6-Tri-Me ether: [78134-85-7]. *5,7-Dihydroxy-3′,4′,7-trimethoxyisoflavone.* ***Junipegenin B.*** *Dalspinosin*
$C_{18}H_{16}O_7$ M 344.320
Isol. from leaves of *Juniperis macropoda* and roots of *Dalbergia spinosa*. Golden-yellow plates (MeOH). Mp 188-189°.

4′,5-Di-Me, 6,7-methylenedioxy ether: [69618-04-8]. *3′-Hydroxy-4′,5-dimethoxy-6,7-methylenedioxyiosflavone.* ***Iriskumaonin***
$C_{18}H_{14}O_7$ M 342.304
Isol. from *I. kumaonensis, I. germanica* and *I. tingitana*. Minute prisms (MeOH), silky solid (EtOAc/pet. ether). Mp 207-208° (203-205°).

6-Me, 3′,4′-methylene ether: [83162-85-0]. *5,7-Dihydroxy-6-methoxy-3′,4′-methylenedioxyisoflavone.* ***Dalspinin***
$C_{17}H_{12}O_7$ M 328.278
Obt. from roots of *Dalbergia spinosa*. Mp 200-202°.

5,6-Di-Me, 3′,4′-methylenedioxy ether: [68862-19-1]. *7-Hydroxy-5,6-dimethoxy-3′,4′-methylenedioxyisoflavone.* ***Isoplatycarpanetin.*** *Dipteryxin*†
$C_{18}H_{14}O_7$ M 342.304
Isol. from *Cladrastis platycarpa, C. shikokiana* and *Dipteryx odorata*. Cryst. ($CHCl_3/Et_2O$). Mp 235-237°. The name Dipteryxin has also been given to 7,8-Dihydroxy-4′,6-dimethoxyisoflavone from *D. odorata* therefore the name Isoplatycarpanetin is preferred here.

5,6-Di-Me, 3′,4′-methylenedioxy ether, 7-O-β-D-glucopyranoside:
$C_{24}H_{24}O_{12}$ M 504.446
Isol. from *Cladrastis platycarpa* and *C. shikokiana*.

5,6,7-Tri-Me, 3′,4′-methylenedioxy ether: [51986-39-1]. *5,6,7-Trimethoxy-3′,4′-methylenedioxyisoflavone.* ***Odoratine***†
$C_{19}H_{16}O_7$ M 356.331
Isol. from *Cordyla africana* and *Dipteryx odorata*. Cryst. ($CHCl_3/Et_2O$). Mp 172-174°. The name Odoratin(e) has also been used for 3′,7-Dihydroxy-4′,6-dimethoxyisoflavone from *D.* spp., and additionally for at least 3 other nat. prods.

[86849-77-6]

Morita, N. *et al, Chem. Pharm. Bull.*, 1972, **20**, 730 (*Iristectorigenin A*)
Arisawa, M. *et al, Chem. Pharm. Bull.*, 1973, **21**, 600, 2323 (*Iristectorigenin B*)
Campbell, R.V.M. *et al, J. Chem. Soc., Perkin Trans.* 1, 1973, 2222 (*Dalspinin*)
Antus, S. *et al, Chem. Ber.*, 1975, **108**, 3883 (*synth, pmr*)
Kalla, A.K. *et al, Phytochemistry*, 1978, **17**, 1441 (*Iriskumaonin*)
Nakano, T. *et al, J. Chem. Soc., Perkin Trans.* 1, 1979, 2107 (*Odoratine, Dipteryxine*)
Sethi, M.L. *et al, Phytochemistry*, 1981, **20**, 341 (*Junipegenin B*)
Dasan, R.G. *et al, Indian J. Chem., Sect. B*, 1982, **21**, 385 (*Junipegenin B*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Sethi, M.L. *et al, Phytochemistry*, 1983, **22**, 289 (*synth*)
Shawl, A.S. *et al, Phytochemistry*, 1984, **23**, 2405 (*isol*)

3′,4′,5′,6,7-Pentahydroxyisoflavone P-80044

Updated Entry replacing T-03614

*6,7-Dihydroxy-3-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one*
$C_{15}H_{10}O_7$ M 302.240

3′,6,7-Tri-Me, 4′,5′-methylenedioxy ether: [24203-70-1]. *3′,6,7-Trimethoxy-4′,5′-methylenedioxyisoflavone*
$C_{19}H_{16}O_7$ M 356.331
Constit. of *Cordyla africana* and *Mildbraeodendron excelsa* heartwoods. Needles (MeOH). Mp 211-212°.

Penta-Me ether: [58523-19-6]. *3′,4′,5′,6,7-Pentamethoxyisoflavone*
$C_{20}H_{20}O_7$ M 372.374
Isol. from trunkwood of *Pterodon apparicioi*. Mp 210-212°.

Campbell, R.V.M. *et al*, *J. Chem. Soc. C*, 1969, 1787 (*isol, ir, uv, pmr, ms*)
Meegan, M.J. *et al*, *Phytochemistry*, 1975, **14**, 2283 (*isol*)
Leite de Almeida, M.E. *et al*, *Phytochemistry*, 1975, **14**, 2716 (*isol*)

3′,4′,5,7,8-Pentahydroxyisoflavone P-80045

Updated Entry replacing T-01267

*3-(3,4-Dihydroxyphenyl)-5,7,8-dihydroxy-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{10}O_7$ M 302.240

Prod. by *Aspergillus niger* and *Streptomyces neyagawaensis* var. *orobolare*. DOPA decarboxylase inhibitor. Brownish cryst. (MeOH/C_6H_6). Mp 252° dec.

8-Me ether: [58262-89-8]. *3′,4′,5,7-Tetrahydroxy-8-methoxyisoflavone. 8-Methoxyorobol*
$C_{16}H_{12}O_7$ M 316.267
Isol. from cultures of *Aspergillus niger*. DOPA decarboxylase inhibitor. Brownish cryst. (MeOH/C_6H_6). Mp 252° dec. All isolations of isoflavones from microorganisms are considered dubious.

3′,8-Di-Me ether: [41744-53-0]. *4′,5,7-Trihydroxy-3′,8-dimethoxyisoflavone. Homotectorigenin*
$C_{17}H_{14}O_7$ M 330.293
Not yet isol. from nature.

3′,8-Di-Me ether, 7-O-glucoside: [41744-52-9]. ***Homotectoridin***
$C_{23}H_{24}O_{12}$ M 492.435
Isol. from rhizomes of *Iris germanica*. Needles (EtOH aq.). Mp 186°.

4′,8-Di-Me ether: [56419-18-2]. *3′,5,7-Trihydroxy-4′,8-dimethoxyisoflavone*
$C_{17}H_{14}O_7$ M 330.293
Isol. from *Monopteryx inpae* and from cultures of *Streptomyces* sp. All isolations of isoflavones from microorganisms are considered dubious.

3′,4′,8-Tri-Me ether: [78182-91-9]. *5,7-Dihydroxy-3′,4′,8-trimethoxyisoflavone*
$C_{18}H_{16}O_7$ M 344.320
Isol. from trunkwood of *M. inpae*. Yellow cryst. Mp 168-169°.

5,8-Di-Me, 3′,4′-methylene ether: [53505-60-5]. *7-Hydroxy-5,8-dimethoxy-3′,4′-methylenedioxyisoflavone.* ***Platycarpanetin***
$C_{18}H_{14}O_7$ M 342.304
Isol. from *Cladrastis platycarpa* and *C. shikokiana*.

5,8-Di-Me, 3′,4′-methylene ether, 7-O-glucoside: [52783-55-8]. *Platycarpanetin 7-O-glucoside*
$C_{24}H_{24}O_{12}$ M 504.446
Isol. from *C. platycarpa* and *C. shikokiana*. Needles. Mp 142-144°.

5,8-Di-Me, 3′,4′-methylene ether, 7-O-laminaribioside: Platycarpanetin 7-O-laminaribioside
$C_{30}H_{34}O_{17}$ M 666.588
Isol. from *C. platycarpa* and *C. shikokiana*. Struct. of glycoside residue not certain.

Penta-Me ether: [57800-12-1]. *3′,4′,5,7,8-Pentamethoxyisoflavone*
$C_{20}H_{20}O_7$ M 372.374
Mp 167-169° (163°).

Kawase, A. *et al*, *Agric. Biol. Chem.*, 1973, **37**, 145.
Imamura, H. *et al*, *Phytochemistry*, 1974, **13**, 757 (*Platycarpanetin*)
Chimura, H. *et al*, *J. Antibiot.*, 1975, **28**, 619 (*isol*)
Umezawa, H. *et al*, *J. Antibiot.*, 1975, **28**, 947 (*isol*)
Tobe, H. *et al*, *J. Antibiot.*, 1976, **29**, 623 (*isol*)
Albuquerque, F.B. *et al*, *Phytochemistry*, 1981, **20**, 235 (*5,7-Dihydroxy-3′,4′,8-trimethoxyisoflavone*)

3′,4′,6,7,8-Pentahydroxyisoflavone P-80046

Updated Entry replacing T-20284

*3-(3,4-Dihydroxyphenyl)-6,7,8-trihydroxy-4*H*-1-benzopyran-4-one*

$C_{15}H_{10}O_7$ M 302.240

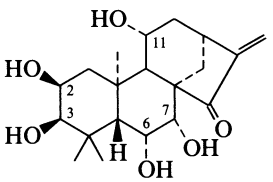
4′,7,8-Tri-Me ether: 3′,8-Dihydroxy-4′,7,8-trimethoxyisoflavone
$C_{18}H_{16}O_7$ M 344.320
Isol. from cultures of *Streptomyces* sp. All isolations of isoflavonoids from microorganisms are considered dubious.

6,7,8-Tri-Me, 3′,4′-methylenedioxy ether: [71339-42-9]. *6,7,8-Trimethoxy-3′,4′-methylenedioxyisoflavone.* ***Petalostetin***
$C_{19}H_{16}O_7$ M 356.331
Isol. from *Petalostemon candidum*. Needles (EtOAc/pet. ether). Mp 169-170°.

3′,4′,8-Tri-Me, 6,7-methylenedioxy ether: 3′,4′,8-Trimethoxy-6,7-methylenedioxyisoflavone
$C_{19}H_{16}O_7$ M 356.331
Isol. from *Xanthocercis zambesiaca*. Probable struct. Not obt. pure.

Chimura, H. *et al*, *J. Antibiot.*, 1975, **28**, 619 (*3′,8-Dihydroxy-4′,7,8-trimethoxyisoflavone*)
Harper, S.H. *et al*, *Phytochemistry*, 1976, **15**, 1019 (*3′,4′,8-Trimethoxy-6,7-methylenedioxyisoflavone*)
Torrance, S.J. *et al*, *Phytochemistry*, 1979, **18**, 366 (*Petalostetin*)
Bhardwaj, D.K. *et al*, *Indian J. Chem., Sect. B*, 1982, **21**, 493 (*synth, Petalostetin*)

ent-2α,3α,6β,7β,11β-Pentahydroxy-16-kauren-15-one P-80047



$C_{20}H_{30}O_6$ M 366.453

2,3,6,11-Tetra-Ac: [93078-70-7]. ent-2α,3α,6β,11β-*Tetraacetoxy-7β-hydroxy-16-kauren-15-one.* ***Lushanrubescensin***
$C_{28}H_{38}O_{10}$ M 534.602
Isol. from leaves of *Rabdosia rubescens*.

7-Epimer, 2,3,6-tri-Ac: [110325-77-4]. ent-2α,3α,6β-*Triacetoxy-7α,11β-dihydroxy-16-kauren-15-one.* ***Lushanrubescensin B***
$C_{26}H_{36}O_8$ M 476.566
Isol. from *R. rubescens*.

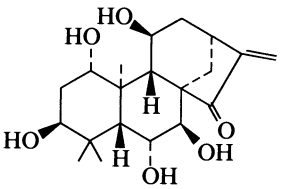
7-Deoxy, 3-Ac: [110325-79-6]. ent-3α-*Acetoxy-2α,6β,11β-trihydroxy-16-kauren-15-one.* ***Lushanrubescensin D***
$C_{22}H_{32}O_6$ M 392.491
Isol. from *R. rubescens*.

7-Deoxy, 3,6-Di-Ac: ent-3α,6β-*Diacetoxy-2α,11β-dihydroxy-16-kauren-15-one.* ***Lushanrubescensin E***
$C_{24}H_{34}O_7$ M 434.528
Isol. from *Rabdosia rubescens*, f. *lushanensis*. Shows antineoplastic props.

7-Deoxy, tetra-Ac: [110325-78-5]. ent-2α,3α,6β,11β-*Tetraacetoxy-16-kauren-15-one.* ***Lushanrubescensin C***
$C_{28}H_{38}O_9$ M 518.603
Isol. from *R. rubescens*.

Qin, C. *et al*, *CA*, 1984, **101**, 226852v; 1987, **107**, 130873a, 130874b.
Li, J. *et al*, *CA*, 1988, **108**, 164740r.

ent-1β,3α,6β,7α,11α-Pentahydroxy-16-kauren-15-one P-80048



$C_{20}H_{30}O_6$ M 366.453

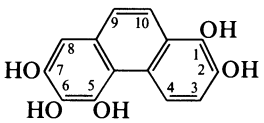
1,7,11-Tri-Ac: ***Weisiensin A***
$C_{26}H_{36}O_9$ M 492.565
Constit. of *Rabdosia weisiensis*. Needles. Mp 298-300°.

Yunlong, X. *et al*, *Phytochemistry*, 1989, **28**, 1978.

1,2,5,6,7-Pentahydroxyphenanthrene P-80049

Updated Entry replacing P-60050

1,2,5,6,7-Phenanthrenepentol



$C_{14}H_{10}O_5$ M 258.230

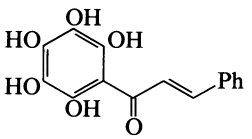
1,5,6-Tri-Me ether: [108909-02-0]. *1,5,6-Trimethoxy-2,7-phenanthrenediol, 9CI.* 2,7-*Dihydroxy*-1,5,6-*trimethoxyphenanthrene.* ***Confusarin***
$C_{17}H_{16}O_5$ M 300.310
Constit. of *Eria confusa*. Cryst. (EtOAc/pet. ether). Mp 185°.

1,5,7-Tri-Me ether: 1,5,7-Trimethoxy-2,6-phenanthrenediol. 2,6-Dihydroxy-1,5,7-trimethoxyphenanthrene
$C_{17}H_{16}O_5$ M 300.310
Constit. of *Eulophia nuda*. Plates (CH_2Cl_2). Mp 152-153°.

Majumder, P.L. *et al*, *Phytochemistry*, 1987, **26**, 1127 (*isol*)
Tuchinda, P. *et al*, *Phytochemistry*, 1988, **27**, 3267 (*isol*)

1-(2,3,4,5,6-Pentahydroxyphenyl)-3-phenyl-2-propen-1-one P-80050

2′,3′,4′,5′,6′-Pentahydroxychalcone



$C_{15}H_{12}O_6$ M 288.256

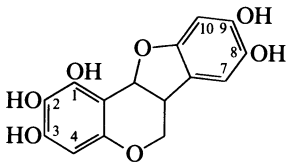
2′,4′,5′-Tri-Me ether: [521-51-7]. *1-(2,5-Dihydroxy-3,4,6-trimethoxyphenyl)-3-phenyl-2-propen-1-one. 2′,5′-Dihydroxy-3′,4′,6′-trimethoxychalcone.* ***Pedicin***
$C_{18}H_{18}O_6$ M 330.337
Isol. from leaves of *Didymocarpus pedicellata* and in various Gesneraceae spp. Orange-red cryst. (Et_2O). Mp 143-145°.

Penta-Me ether: [518-58-1]. *1-(2,3,4,5,6-Pentamethoxyphenyl)-3-phenyl-2-propen-1-one. 2′,3′,4′,5′,6′-Pentamethoxychalcone.* ***Pedicellin***†
$C_{20}H_{22}O_6$ M 358.390
Isol. from leaves of *D. pedicellata* and in various Gesneraceae spp. Tablets or needles (Et_2O or pet. ether). Mp 93°.

[27619-60-9]

Siddiqui, S., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1939, 673 (*isol*)
Baker, W., *J. Chem. Soc.*, 1941, 662 (*synth*)
Seshadri, J.R., *J. Indian Chem. Soc.*, 1965, **42**, 343 (*struct, synth, Pedicin*)
Harborne, J.B., *Phytochemistry*, 1966, **5**, 589 (*occur*)

1,2,3,8,9-Pentahydroxypterocarpan P-80051

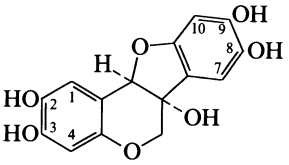


$C_{15}H_{12}O_7$ M 304.256

2-Me, 8,9-methylene ether: [73520-83-9]. *1,3-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan.* ***Trifolian***
$C_{17}H_{14}O_7$ M 330.293
Isol. from roots of *Trifolium pratense*. Cryst. (MeOH). Mp 132-134°. $[\alpha]_D$ −240° (c, 0.5 in MeOH).

Fraishtat, P.D. *et al*, *Bioorg. Khim.*, 1979, **5**, 1879; 1981, **7**, 927.

2,3,6*a*,8,9-Pentahydroxypterocarpan P-80052



$C_{15}H_{12}O_7$ M 304.256

2,3-Di-Me, 8,9-methylene ether: [83159-18-6]. *6a-Hydroxy-2,3-dimethoxy-8,9-methylenedioxypterocarpan.* ***Lathycarpin***
$C_{18}H_{16}O_7$ M 344.320
Phytoalexin from leaves of *Lathyrus sativus*. $[\alpha]_D^{21}$ +232° (c, 0.012 in MeOH).

Ingham, J.L. *et al*, *Z. Naturforsch., C*, 1982, **37**, 724 (*isol, uv, pmr, struct, abs config*)

3,4,6*a*,8,9-Pentahydroxypterocarpan P-80053

Updated Entry replacing A-20005

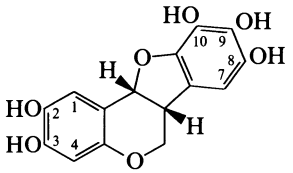
$C_{15}H_{12}O_7$ M 304.256

3,4:8,9-Bismethylene ether: [70285-12-0]. *6a-Hydroxy-3,4:8,9-bis(methylenedioxy)pterocarpan.* ***Acanthocarpan***
$C_{17}H_{12}O_7$ M 328.278
Stress metab. from leaves of *Caragana acanthophylla* and *Tephrosia bidwilli*. $[\alpha]_D$ −259° (c, 0.23 in MeOH). Revised struct.

4-Me, 8,9-Methylene ether: [87402-98-0]. *3,6a-Dihydroxy-4-methoxy-8,9-methylenedioxypterocarpan.* ***Tephrocarpin***
Stress metab. from leaves of *T. bidwilli*. $[\alpha]_D$ −267° (c, 0.04 in MeOH).

Ingham, J.L. *et al*, *Phytochemistry*, 1982, **21**, 2969.

2,3,8,9,10-Pentahydroxypterocarpan P-80054



Absolute configuration

$C_{15}H_{12}O_7$ M 304.256

3,9,10-Tri-Me ether: [76474-66-3]. ***2,8-Dihydroxy-3,9,10-trimethoxypterocarpan***
$C_{18}H_{18}O_7$ M 346.336
Isol. from *Swartzia laevicarpa* trunkwood. Cryst. (C_6H_6/Me_2CO). Mp 126-127°.

Braz Filho, R. *et al*, *Phytochemistry*, 1980, **19**, 2003 (*isol, ir, uv, pmr, cmr, struct*)

3,4,8,9,10-Pentahydroxypterocarpan P-80055

$C_{15}H_{12}O_7$ M 304.256

3,4,9,10-Tetra-Me ether: [89675-59-2]. *8-Hydroxy-3,4,9,10-tetramethoxypterocarpan*
$C_{19}H_{20}O_7$ M 360.363
Isol. from trunkwood of *Swartzia laevicarpa*. Cryst. (C_6H_6/pet. ether). Mp 196-198°.

3,4,9,10-Tetra-Me ether, Ac: [89675-60-5].
Cryst. (pet. ether). Mp 192-194°.

Braz Filho, R. *et al*, *Phytochemistry*, 1980, **19**, 2003 (*isol, pmr, ord, ms, struct*)

3,6*a*,7,8,9-Pentahydroxypterocarpan P-80056

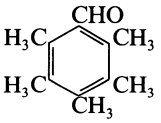
$C_{15}H_{12}O_7$ M 304.256

*8,9-Methylene ether: 3,6*a*,7-Trihydroxy-8,9-methylenedioxypterocarpan.* 6a,7-*Dihydroxymaackiain*
$C_{16}H_{12}O_7$ M 316.267
Isol. from fungus-infected leaves of *Trifolium pratense*.

Ingham, J.L., *Phytochemistry*, 1976, **15**, 1489.

Pentamethylbenzaldehyde P-80057

[17432-38-1]



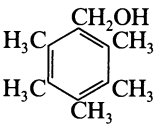
$C_{12}H_{16}O$ M 176.258
Cryst. (hexane). Mp 148-150°.

Wasserman, H.H. *et al*, *J. Org. Chem.*, 1971, **36**, 1765 (*synth, ir, pmr, ms*)
Bjørgo, J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1977, 254 (*synth*)

Pentamethylbenzyl alcohol P-80058

2,3,4,5,6-Pentamethylbenzenemethanol, 9CI

[484-66-2]



$C_{12}H_{18}O$ M 178.274
Cryst. (C_6H_6/hexane). Mp 162-163°.

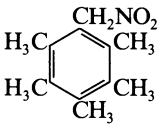
Ac: [19936-85-7].
$C_{14}H_{20}O_2$. Cryst. Mp 85°.

Wasserman, H.H. *et al*, *J. Org. Chem.*, 1971, **36**, 1765 (*synth, ir, pmr, ms*)
Baciocchi, E. *et al*, *J. Org. Chem.*, 1977, **42**, 3682 (*deriv, pmr*)
Rudenko, A.P. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1985, **21**, 1609 (*synth, deriv, pmr*)

Pentamethyl(nitromethyl)benzene, 9CI P-80059

Pentamethylphenylnitromethane

[29328-77-6]



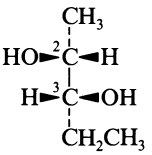
$C_{12}H_{17}NO_2$ M 207.272
Prisms (pet.ether). Mp 86-88°.

Suzuki, H., *Bull. Chem. Soc. Jpn.*, 1970, **43**, 879 (*synth, ir, pmr*)
Chiba, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 2614 (*synth*)
Kim, E.K. *et al*, *J. Org. Chem.*, 1989, **54**, 1692 (*synth, ir, pmr*)

2,3-Pentanediol, 9CI P-80060

Updated Entry replacing P-00478

[42027-23-6]



(2*RS*,3*RS*)-*form*

$C_5H_{12}O_2$ M 104.149

(2RS,3RS)-form [61828-36-2]
(±)-threo-*form*
Liq. d_4^{25} 0.965. Bp_{10} 83°. n_D^{20} 1.4320.

Bis(4-methylbenzenesulfonyl): Cryst. (Et_2O/pentane). Mp 88-89°.

Di-Ac:
$C_9H_{16}O_4$ M 188.223
Bp_{10} 89°. n_D^{20} 1.4195.

(2RS,3SR)-form [61828-35-1]
(±)-*erythro-form*
Liq. d_4^{25} 0.978. Bp_{10} 89°. n_D^{20} 1.4431.

Bis(4-methylbenzenesulfonyl): Cryst. (pentane). Mp 81.5-83°.

Di-Ac: Bp_{10} 85°. n_D^{20} 1.4167.

[97847-54-6, 97847-55-7]

Lucas, H.J. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 22 (*synth*)
Emmons, W.D. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 3472 (*synth*)
Rebrovic, L. *et al*, *J. Org. Chem.*, 1984, **49**, 2462 (*synth*)

4-Pentyn-1-amine, 9CI P-80061

4-Pentynylamine, 8CI. 5-Amino-1-pentyne

[15252-44-5]

$HC{\equiv}CCH_2CH_2CH_2NH_2$

C_5H_9N M 83.133
Bp 124°.

Dumont, J.-L. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 588 (*synth, ir*)

4-Pentynoic acid, 9CI P-80062

Updated Entry replacing P-00592

[6089-09-4]

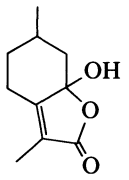
$HC{\equiv}CCH_2CH_2COOH$

$C_5H_6O_2$ M 98.101
Cryst. Mp 57°.
▷ SC4751000.
Me ester: [21565-82-2].
$C_6H_8O_2$ M 112.128
Bp 143-144°, Bp_{175} 101-102°.
p-*Bromophenacyl ester:* Long needles. Mp 103°.

Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1954, 797 (*synth*)
Schulte, K.E. *et al*, *Chem. Ber.*, 1954, **87**, 964 (*synth*)
Holland, B.C. *et al*, *Synth. Commun.*, 1974, **4**, 203 (*synth, ir, pmr*)
Martel, J. *et al*, *Bull. Soc. Chim. Fr.*, 1978, 131 (*synth*)
Wulff, W.D. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 7419 (*synth, pmr*)

Peperinic acid P-80063

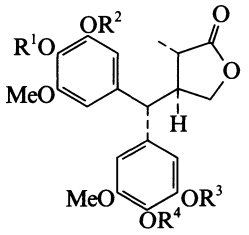
Updated Entry replacing H-00678
2,4,5,6,7,7a-Hexahydro-7a-hydroxy-3,6-dimethyl-2-benzofuranone
[514-93-2]



$C_{10}H_{14}O_3$ M 182.219
Constit. of *Bursera graveolens* and *Bystropogon mollis*. Also isol. from aged peppermint oil. Cryst. (MeOH or C_6H_6). Mp 191° (188-189°). $[\alpha]_D^{21}$ +60.7°. Prob. artifact of oxidn.

Fester, G.A. *et al*, *An. Asoc. Quim. Argent.*, 1949, **37**, 197; 1952, **40**, 246; *CA*, **40**, 4636; **48**, 1974 (*isol*)
Woodward, R.B. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 399 (*isol*)
Crowley, K.J. *et al*, *J. Chem. Soc.*, 1964, 4254 (*isol*)

Peperomin A P-80064



$R^1R^2 = R^3R^4 = -CH_2-$

$C_{22}H_{22}O_8$ M 414.411
Constit. of *Peperoma japonica*. Cryst. (MeOH aq.). Mp 143-145°. $[\alpha]_D^{27}$ +20.6° (c, 0.136 in $CHCl_3$).

Chen, C.-M. *et al*, *Heterocycles*, 1989, **29**, 411.

Peperomin B P-80065

As Peperomin A, P-80064 with

$R^1 = R^2 = Me$, $R^3R^4 = -CH_2-$

$C_{23}H_{26}O_8$ M 430.454
Constit. of *Peperoma japonica*. Cryst. (MeOH aq.). Mp 143-145°. $[\alpha]_D^{27}$ +28.9° (c, 0.444 in $CHCl_3$).

Chen, C.-M. *et al*, *Heterocycles*, 1989, **29**, 411 (*isol, cryst struct*)

Peperomin C P-80066

As Peperomin A, P-80064 with

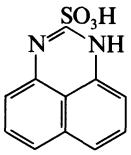
$R^1 = R^2 = R^3 = R^4 = Me$

$C_{24}H_{30}O_8$ M 446.496
Constit. of *Peperoma japonica*. Cryst. (MeOH). Mp 158-160°. $[\alpha]_D^{27}$ +42.7° (c, 0.059 in $CHCl_3$).

Chen, C.-M. *et al*, *Heterocycles*, 1989, **29**, 411.

1*H*-Perimidine-2-sulfonic acid P-80067

[110448-71-0]

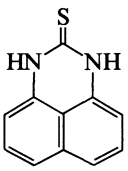


$C_{11}H_8N_2O_3S$ M 248.262
Pale yellow needles. Mp >300°.

Herbert, J.M. *et al*, *Heterocycles*, 1987, **26**, 1043 (*synth, ir, pmr*)

1*H*-Perimidine-2(3*H*)-thione, 9CI P-80068

Updated Entry replacing P-10051
3H-Benzo[de]*quinazoline-2-thione. 2-Mercapto-1H-perimidine*
[30837-62-8]

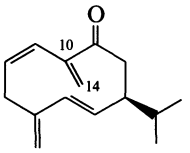


$C_{11}H_8N_2S$ M 200.264
Thione-form (shown) predominates. Readily obt. from 1,8-naphthalenediamine and CS_2 in 95% yield. Cryst. ($CHCl_3$). Mp 265° dec.
S-*Me:* [92972-05-9]. *2-(Methylthio)perimidine*
$C_{12}H_{10}N_2S$ M 214.290
Yellow prisms (Me_2CO). Mp 199-200.5°.
S-*Me; B,HI:* [89473-00-7].
Yellow cryst. Mp >300°.
S-*Me*, S-*oxide:* [110191-88-3]. *2-(Methylsulfinyl)perimidine*
$C_{12}H_{10}N_2OS$ M 230.290
Yellow needles by subl. Mp 181-182°.

Liu, K.-C. *et al*, *Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 928.
Liu, J. *et al*, *J. Heterocycl. Chem.*, 1984, **21**, 911 (*synth, uv, ir, ms*)
Liu, K.-C. *et al*, *J. Heterocycl. Chem.*, 1984, **21**, 911 (*synth, deriv, bibl*)
Herbert, J.M. *et al*, *J. Med. Chem.*, 1987, **30**, 2081 (*synth, deriv, pmr, ms*)

Periplanone D_1 P-80069

[123163-72-4]



$C_{15}H_{20}O$ M 216.322
Constit. of faeces of female cockroaches *Periplaneta americana*.
10S,14-Dihydro: [123062-72-6]. ***Periplanone D_2***

$C_{15}H_{22}O$ M 218.338
Metab. of *P. americana*.

[111917-97-6]

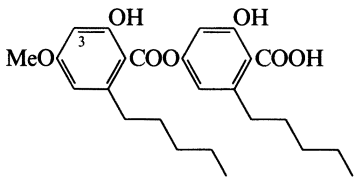
Biendl, M. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2367.

Perlatolic acid P-80070

Updated Entry replacing P-00637

2-Hydroxy-4-[(2-hydroxy-4-methoxy-6-pentylbenzoyl)oxy]-6-pentylbenzoic acid, 9CI. Perlatolinic acid

[529-47-5]



$C_{25}H_{32}O_7$ M 444.524
Constit. of many lichens including *Cladonia evansii* and *Ramalina stenospora*. Needles (C_6H_6). Mp 108°.

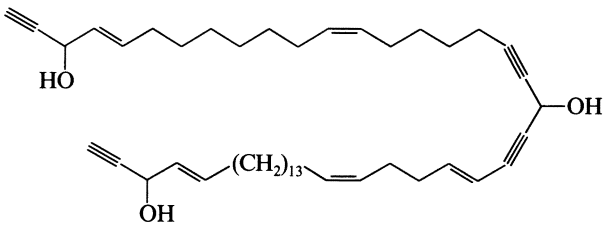
Di-Me ether, Me ester: Needles (MeOH). Mp 57°.

Benzyl ester: [53530-28-2].
Needles (pentane). Mp 56.5-57°.

3-Chloro: [120091-97-6]. ***3-Chloroperlatolic acid***
$C_{25}H_{31}ClO_7$ M 478.968
Constit. of *Dimelaena calcifornica*. Cryst. (EtOAc/pet. ether). Mp 128°.

Elix, J.A. *et al*, *Aust. J. Chem.*, 1974, **27**, 1767 (*synth, pmr, ms, bibl*)
Elix, J.A. *et al*, *Aust. J. Chem.*, 1988, **41**, 1789 (*isol, struct, synth*)

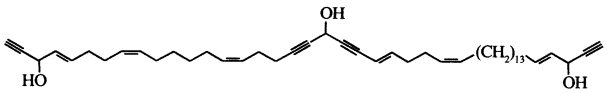
Petroformyne 1 P-80071



$C_{46}H_{68}O_3$ M 669.041
Constit. of *Petrosia ficiformis*. Cytotoxic, inhibits sea urchin egg development. $[\alpha]_D^{25}$ +12.5° (c, 10 in $CHCl_3$).

Cimino, G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3563.

Petroformyne 2 P-80072



$C_{46}H_{66}O_3$ M 667.026
Constit. of *Petrosia ficiformis*. Cytotoxic, inhibits sea urchin egg development. $[\alpha]_D^{25}$ +15° ($CHCl_3$).

Cimino, G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3563.

Petroformyne 3 P-80073

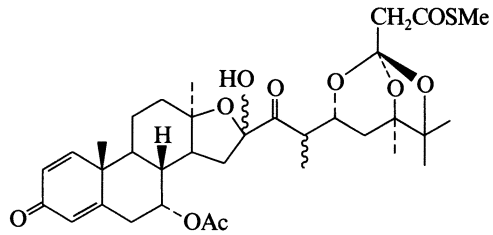
$C_{46}H_{70}O_2$ M 655.058
Constit. of *Petrosia ficiformis*. Cytotoxic, inhibits sea urchin egg development. $[\alpha]_D$ +10.0° ($CHCl_3$).

43Z,44-Didehydro: ***Petroformyne 4***
$C_{46}H_{68}O_2$ M 653.042
Constit. of *P. ficiformis*. Cytotoxic, inhibits sea urchin egg development. $[\alpha]_D$ +6.0° ($CHCl_3$).

Cimino, G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3563.

Petuniasterone N P-80074

[123458-54-8]



$C_{34}H_{46}O_{10}S$ M 646.797
Constit. of *Petunia* spp.

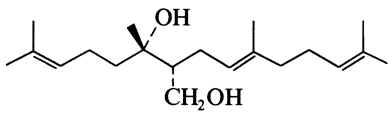
Elliger, C.A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 576 (*isol, pmr, cmr*)

Peucelinendiol P-80075

Updated Entry replacing P-00678

7-Hydroxymethyl-2,6,10,14-tetramethyl-2,9E,13E-pentadecatrien-6-ol

[72776-48-8]



$C_{20}H_{36}O_2$ M 308.503
Constit. of *Peucedanum oreoselinum*. Oil. $[\alpha]_D^{24}$ +5.5° (c, 1.2 in $CHCl_4$).

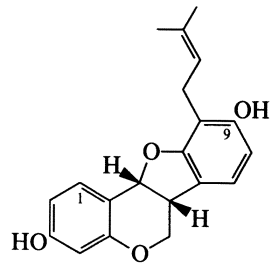
Lemmich, E., *Phytochemistry*, 1979, **18**, 1195 (*isol*)
Moran, J.R. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 4435 (*synth, struct*)

Phaseollidin P-80076

Updated Entry replacing P-00709

6a,11a-Dihydro-10-(3-methyl-2-butenyl)-6H-benzofuro[3,2-c][1]benzopyran-3,9-diol, 9CI. 3,9-Dihydroxy-10-prenylpterocarpan

[37831-70-2]



Absolute configuration

$C_{20}H_{20}O_4$ M 324.376

Isol. from *Phaseolus vulgaris*, *P. aureus*, *P. calcaratus*, *Dolichos biflorus*, *Erythrina abyssinica*, *E. crista-galli*, *E. sandwicensis*, *Lablab niger*, *Macroptilium atropurpureum*, *Psophocarpus tetragonolobus* and *Vigna unguiculata* (all Leguminosae, Papilionoideae). Antifungal antibiotic. Green bean phytoalexin. Mp 67-69°.

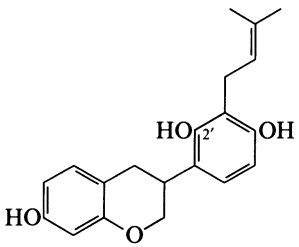
9-Me ether: [74515-46-1]. ***Sandwicensin***
$C_{21}H_{22}O_4$ M 338.402
Isol. from leaves of *Erythrina sandwicensis*. $[\alpha]_D$ −190° (c, ca. 0.02 in MeOH).

1-Methoxy: [65428-13-9]. ***1-Methoxyphaseollidin.*** *3,9-Dihydroxy-1-methoxy-10-prenylpterocarpan*
$C_{21}H_{22}O_5$ M 354.402
Isol. from seeds of *Psophocarpus tetragonolobus*. $[\alpha]_D^{18}$ −225° ($CHCl_3$). Probable struct.

Scheffer, T.C., *Annu. Rev. Phytopathol.*, 1966, **4**, 147 (*rev*)
Perrin, D.R. *et al*, *Tetrahedron Lett.*, 1972, 1673 (*struct, nmr, uv, ms*)
Burden, R.S. *et al*, *Tetrahedron Lett.*, 1972, 4175 (*isol, struct*)
Perrin, D.R. *et al*, *Aust. J. Chem.*, 1974, **27**, 1607 (*struct*)
Preston, N.W., *Phytochemistry*, 1977, **16**, 2044 (1-*Methoxyphaseollidin*)
Ingham, J.L., *Z. Naturforsch., C*, 1980, **35**, 384 (*Sandwicensin*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

Phaseollidinisoflavan P-80077

2′,4′,7-Trihydroxy-3′-prenylisoflavan



$C_{20}H_{22}O_4$ M 326.391

2′-Me ether: [56257-28-4]. ***2′-O-Methylphaseollidinisoflavan***
$C_{21}H_{24}O_4$ M 340.418
Isol. from stems of *Vigna unguiculata*.

Preston, N.W., *Phytochemistry*, 1975, **14**, 1131 (*isol, pmr, struct*)

1,8-Phenanthrenedicarboxylic acid P-80078

[59795-49-2]
$C_{16}H_{10}O_4$ M 266.253
Cryst. (AcOH). Mp 365° dec.

Di-Me ester: [73049-18-0].
$C_{18}H_{14}O_2$ M 262.307
Cryst. (MeOH). Mp 146-147°.

[38378-77-7]

Rubin, M.B. *et al*, *J. Org. Chem.*, 1980, **45**, 1847 (*synth, uv, ir, pmr*)

9-Phenanthrenemethanol, 9CI P-80079

Updated Entry replacing P-00778

9-Hydroxymethylphenanthrene. 9-Phenanthrylcarbinol

[4707-72-6]
$C_{15}H_{12}O$ M 208.259
Needles (C_6H_6/pet. ether). Mp 149-149.5°.

Ac: [53440-11-2].
$C_{17}H_{14}O_2$ M 250.296
Needles (hexane). Mp 79-80°.

Bachmann, W.E., *J. Am. Chem. Soc.*, 1934, **56**, 1366 (*synth*)
Fernández, F. *et al*, *Synthesis*, 1988, 802 (*synth, ir, pmr*)

2,4,7-Phenanthrenetriol P-80080

Updated Entry replacing P-20086

2,4,7-Trihydroxyphenanthrene

$C_{14}H_{10}O_3$ M 226.231

Tri-Me ether: [53077-33-1]. *2,4,7-Trimethoxyphenanthrene*
$C_{17}H_{16}O_3$ M 268.312
Mp 113-114°.

2-Me ether, 9,10-dihydro: [87530-30-1]. *9,10-Dihydro-7-methoxy-2,5-phenanthrenediol. 4,7-Dihydroxy-2-methoxy-9,10-dihydrophenanthrene*
$C_{15}H_{14}O_3$ M 242.274
Obt. from *Bletilla striata*. Shows antimicrobial props. Needles (Me_2CO). Mp 72°.

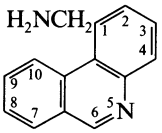
4-Me ether, 9,10-dihydro: 9,10-Dihydro-4-methoxy-2,7-phenanthrenediol. 2,7-Dihydroxy-4-methoxy-9,10-dihydrophenanthrene. ***Coelonin***
$C_{14}H_{12}O_3$ M 228.247
Constit. of *Coelogyne ochracea*, *C. elata* and *Eulophia nuda*. Amorph. powder or needles ($CHCl_3$/hexane). Mp 95-96°.

Hardegger, E. *et al*, *Helv. Chim. Acta*, 1963, **46**, 1171; 1974, **57**, 790, 796 (*synth*)
Majumder, P. *et al*, *Phytochemistry*, 1982, **21**, 478 (*deriv*)
Takagi, S. *et al*, *Phytochemistry*, 1983, **22**, 1011 (*deriv*)
Tuchinda, P. *et al*, *Phytochemistry*, 1988, **27**, 3267 (*isol*)

1-Phenanthridenemethanamine P-80081

1-(Aminomethyl)phenanthridine

[120616-63-9]



$C_{14}H_{12}N_2$ M 208.262
Mp 94-96°.

Freter, K.R. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1701 (*synth, pmr*)

4-Phenanthridinemethanamine P-80082

4-(Aminomethyl)phenanthridine

[120616-65-1]
$C_{14}H_{12}N_2$ M 208.262

B,HCl: [120616-66-2].
Cryst. (MeOH). Mp 259-260°.

Freter, K.R. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1701 (*synth, pmr*)

10-Phenanthridinemethanamine P-80083

10-(Aminomethyl)phenanthridine

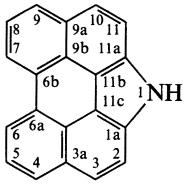
[120616-64-0]
$C_{14}H_{12}N_2$ M 208.262
Cryst. (CH_2Cl_2/pet. ether). Mp 92-93°.

Freter, K.R. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1701 (*synth, pmr*)

1*H*-Phenanthro[1,10,9,8-*cdefg*]carbazole, 9CI **P-80084**

11,12-Iminoperylene

[35337-22-5]



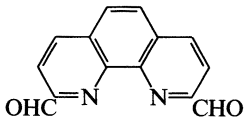
$C_{20}H_{11}N$ M 265.314
Yellow-brown cryst. Mp 360°.

Looker, J.J., *J. Org. Chem.*, 1972, **37**, 3379.

1,10-Phenanthroline-2,9-dicarboxaldehyde **P-80085**

2,9-Diformyl-1,10-phenanthroline

[57709-62-3]



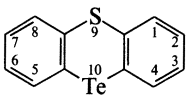
$C_{14}H_8N_2O_2$ M 236.229
Yellow cryst. (THF). Mp 231-232°.

Chandler, C.J. *et al*, *J. Heterocycl. Chem.*, 1981, **18**, 599.
Lüning, U. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 367 (*synth*)

Phenothiatellurin **P-80086**

Thiophenoxtellurine

[262-29-3]

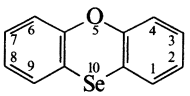


$C_{12}H_8STe$ M 311.861
Light yellow needles (EtOH). Mp 123-124°.

Petragnani, N., *Tetrahedron*, 1960, **11**, 15 (*synth*)
Gioba, A. *et al*, *Rev. Roum. Chim.*, 1970, **15**, 1967 (*synth*)

Phenoxaselenin, 9CI **P-80087**

[262-22-6]



$C_{12}H_8OSe$ M 247.155
Long rectangular prisms with faint floral odour (EtOH or AcOH). Mp 87-88°.

Se-Oxide:
$C_{12}H_8O_2Se$ M 263.154
Cryst. powder. Mp 171-172°. Reforms phenoxaselenin at Mp.

Drew, H.D.K., *J. Chem. Soc.*, 1928, 511 (*synth, derivs*)

4-Phenoxybenzoic acid, 9CI **P-80088**

Updated Entry replacing P-00890

Diphenyl ether 4-carboxylic acid

[2215-77-2]

$C_{13}H_{10}O_3$ M 214.220
Mp 160°. Bp 260°.

Me ester: [21218-94-0].
$C_{14}H_{12}O_3$ M 228.247
Cryst. (EtOH). Mp 60°.

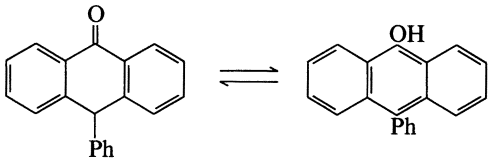
Nitrile: [3096-81-9]. *4-Phenoxybenzonitrile*
$C_{13}H_9NO$ M 195.220
Cryst. solid. Mp 22-24°.

West, R. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 3960 (*ester*)
Manly, D.G. *et al*, *J. Org. Chem.*, 1957, **22**, 323 (*ester*)
Sammes, P.G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 3229 (*nitrile*)

10-Phenylanthrone, 8CI **P-80089**

10-Phenyl-9-anthracenol. 9-Hydroxy-10-phenylanthracene

[14596-70-4]



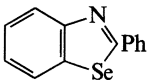
$C_{20}H_{14}O$ M 270.330
Approx. equal amounts of tautomers in soln. Light yellow powder. Mp 139-140°. Readily oxid. by air.

[60079-98-3]

Branz, S.E. *et al*, *Synth. Commun.*, 1986, **16**, 441 (*synth, pmr, tautom*)

2-Phenylbenzoselenazole, 9CI **P-80090**

[32586-68-8]



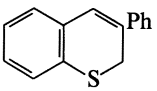
$C_{13}H_9NSe$ M 258.181
Needles (EtOH). Mp 116-117° subl.

Bauer, H., *Ber.*, 1913, **46**, 92 (*synth*)
Croisy, A. *et al*, *Org. Mass Spectrom.*, 1972, **6**, 1321 (*ms*)

3-Phenyl-2*H*-1-benzothiopyran, 9CI **P-80091**

*3-Phenyl-2*H*-1-benzothiin. 3-Phenyl-2*H*-1-thiochromene*

[53844-17-0]



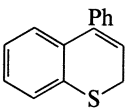
$C_{15}H_{12}S$ M 224.326
Cryst. Mp 64-65°.

Hortmann, A.G. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 6119 (*synth, pmr, ir*)
Arnoldi, A. *et al*, *Synthesis*, 1988, 155 (*synth, pmr*)

4-Phenyl-2*H*-1-benzothiopyran, 9CI **P-80092**

*4-Phenyl-2*H*-thiochromene*

[35813-98-0]



$C_{15}H_{12}S$ M 224.326
Cryst. (MeOH). Mp 83°.

S-Me, perchlorate: [120400-18-2].
$C_{16}H_{15}ClO_4S$ M 338.811

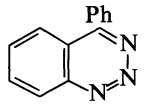
Pale-yellow leaflets. Mp 162-164°.

Lüttringhaus, A. *et al*, *Justus Liebigs Ann. Chem.*, 1962, **654**, 189.
Hori, M. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3816.

4-Phenyl-1,2,3-benzotriazine, 9CI P-80093

Updated Entry replacing P-30088

[33334-16-6]



$C_{13}H_9N_3$ M 207.234

Needles (EtOH). Mp 159-160°. λ_{max} 206, 232 (log ϵ 4.1) and 293 nm (2.95) in EtOH.

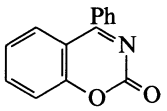
2-Oxide:
$C_{13}H_9N_3O$ M 223.234
Yellow needles (MeOH). Mp 156.5-157.5°.

3-Oxide: [41572-12-7].
$C_{13}H_9N_3O$ M 223.234
Yellow plates (EtOH). Mp 154° dec. Dec. in light.

Meisenheimer, J. *et al*, *Ber.*, 1927, **60**, 1736 (*3-oxide*)
Adger, B.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 31 (*synth, uv, ir*)
Boulton, A.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1509 (*2-oxide*)

4-Phenyl-2*H*-1,3-benzoxazin-2-one, 9CI P-80094

[115438-13-6]



$C_{14}H_9NO_2$ M 223.231

Cryst. Mp 252-255°.

Kamal, A. *et al*, *J. Org. Chem.*, 1988, **53**, 4112 (*synth, ir*)

1-Phenyl-1,3-butadiyne P-80095

1,3-Butadiynylbenzene, 9CI

[5701-81-5]

PhC≡CC≡CH

$C_{10}H_6$ M 126.157

Yellow oil. n_D^{20} 1.6230. Highly unstable to polymerisation.

Negishi, E. *et al*, *J. Org. Chem.*, 1984, **49**, 2629 (*synth*)
Hänninen, E. *et al*, *Acta Chem. Scand., Ser. B*, 1988, **42**, 614 (*synth*)

2-Phenyl-3-butenoic acid, 8CI P-80096

Updated Entry replacing P-50120

α-Ethenylbenzeneacetic acid, 9CI. Phenylvinylacetic acid

[30953-22-1]

$H_2C{=}CHCHPhCOOH$

$C_{10}H_{10}O_2$ M 162.188

(+)-form
Oil. $[\alpha]_D^{25}$ +85.65° (c, 0.704 in EtOH).

(±)-form
Cryst. (pet. ether). Mp 32-33°.

Friedrich, L.E. *et al*, *J. Org. Chem.*, 1971, **36**, 3011 (*synth, uv, ir, pmr*)
Aggarwal, S.K. *et al*, *Tetrahedron*, 1987, **43**, 451 (*resoln*)

4-Phenyl-3-buten-1-ol, 9CI P-80097

Updated Entry replacing P-01064

[937-58-6]

$PhCH{=}CHCH_2CH_2OH$

$C_{10}H_{12}O$ M 148.204

Mp 36°. Bp_{12} 137-138°.

(E)(?)-form
Bp_{12} 137-138°.

Ac: [20473-78-3].
$C_{12}H_{14}O_2$ M 190.241
Bp_{12} 149°.

Phenylurethane: Mp 70°.

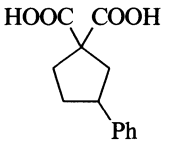
Z-form
Oil. $Bp_{0.15}$ 65° (bulb) .

Methylsulfonyl: Pale orange oil. Bp_1 80° (bulb) .

[7515-42-6]

Hands, A.R. *et al*, *J. Chem. Soc. C*, 1968, 2448 (*synth, pmr*)
Marvell, E.N. *et al*, *Synthesis*, 1973, 457 (*synth*)
Bachi, M.D. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1517 (*synth, ir, pmr, ms*)

3-Phenyl-1,1-cyclopentanedicarboxylic acid P-80098



$C_{13}H_{14}O_4$ M 234.251

(±)-form [115340-09-5]
Needles. Mp 167-169°.

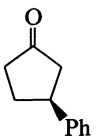
Di-Me ester: [115340-08-4].
$C_{15}H_{18}O_4$ M 262.305
Oil. $Bp_{0.5}$ 145-155° (bulb) .

Grunewald, G.L. *et al*, *J. Org. Chem.*, 1988, **53**, 4021 (*synth, ir, pmr, cmr, ms*)

3-Phenylcyclopentanone, 9CI P-80099

Updated Entry replacing P-01126

[64145-51-3]



(S)-form

$C_{11}H_{12}O$ M 160.215

(S)-form [86505-50-2]
$[\alpha]_D^{25}$ −84.9° (c, 0.72 in $CHCl_3$).

(±)-form
Liq. Bp_{10} 154-155°, Bp_1 120-122°.

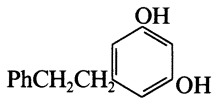
Semicarbazone: Leaflets (EtOH). Mp 181° dec.

Winternitz, F. *et al*, *Bull. Soc. Chim. Fr.*, 1953, 190 (*synth*)
Kolobielski, M. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 5820 (*synth*)
Paquette, L.A. *et al*, *J. Org. Chem.*, 1988, **53**, 4978 (*synth, ir, pmr*)

5-(2-Phenylethyl)-1,3-benzenediol P-80100

5-Phenethylresorcinol, 8CI. 1-(3,5-Dihydroxyphenyl)-2-phenylethane. 3,5-Dihydroxybibenzyl. ***Dihydropinosylvin***

[14531-52-3]



$C_{14}H_{14}O_2$ M 214.263

Prob. trace constit. of *Pinus kremphii* wood. Also in fungus-infected *Dioscorea batatus* as phytoalexin. Oil.

Mono-Me ether: [17635-59-5]. *3-Methoxy-5-(2-phenylethyl)phenol. 3-Hydroxy-5-methoxybibenzyl.* ***Dihydropinosylvin methyl ether***

$C_{15}H_{16}O_2$ M 228.290

Isol. from wood of *P. albicaulis* and other *P.* spp. Mp 50-52°.

Me ether, phenylurethane: Mp 124-125°.

Lindstedt, G., *Acta Chem. Scand.*, 1950, **4**, 1246 (*isol, struct, synth, deriv*)
Erdtman, H. *et al*, *Phytochemistry*, 1966, **5**, 927 (*isol*)
Mitscher, L.A. *et al*, *Phytochemistry*, 1981, **20**, 781 (*synth*)
Takasugi, M. *et al*, *Phytochemistry*, 1987, **76**, 371 (*isol, props*)

7-Phenyl-2,4,6-heptatriyn-1-ol, 9CI P-80101

[60214-15-5]

$PhC{\equiv}CC{\equiv}CC{\equiv}CCH_2OH$

$C_{13}H_8O$ M 180.206

Isol. from *Bidens pilosa* and *B. leucantha*. Shows antimicrobial activity. Cryst. (pet. ether or CCl_4). Mp 66.5° (64°).

Ac: [23414-58-6]. *1-Acetoxy-7-phenyl-2,4,6-heptatriyne*

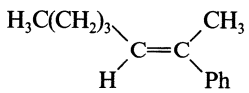
$C_{15}H_{10}O_2$ M 222.243

Isol. from *B. pilosa*, *B. leucantha* and *B. dahlioides*, also in trace amts. from *Coreopsis tinctoria*. Long pale yellow needles (pet. ether). Mp 50°.

Prévost, S. *et al*, *Bull. Soc. Chim. Fr.*, 1961, 2171 (*synth*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 2135; 1965, **98**, 1228; 1966, **99**, 1223 (*isol, uv, ir, pmr*)
Smirnov, V.V. *et al*, *CA*, 1984, **101**, 122607c.

2-Phenyl-2-heptene P-80102

1-Methyl-1-hexenylbenzene, 9CI



$C_{13}H_{18}$ M 174.285

(E)-form [83021-58-3]

Liq. $Bp_{0.01}$ 50-52°.

Brown, H.C. *et al*, *J. Org. Chem.*, 1988, **53**, 6009 (*synth, ir, pmr*)

7-Phenyl-2-heptene-4,6-diynal, 9CI P-80103

[20252-42-0]

$PhC{\equiv}CC{\equiv}CCH{=}CHCHO$

$C_{13}H_8O$ M 180.206

(E)-form [13894-73-0]

Isol. from roots of *Onopordon acanthium*. Yellowish cryst. (pet. ether). Mp 63.5°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3201 (*isol, uv, ir, pmr, synth*)

1-Phenyl-2,4-hexadiyn-1-ol P-80104

α-1,3-Pentadiynylbenzenemethanol, 9CI. Capillol

[1574-95-4]

$PhCH(OH)C{\equiv}CC{\equiv}CCH_3$

$C_{12}H_{10}O$ M 170.210

Ac: O-*Acetylcapillol. Capillol acetate*

$C_{14}H_{12}O_2$ M 212.248

Isol. from roots of *Chrysanthemum frutescens*, *C. foeniculatum* and *Lonas annua*. Oil. λ_{max} 243, 257 nm (ϵ 1230, 830)(Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 39, 602; 1964, **97**, 1179; 1966, **99**, 995, 2413 (*isol, uv, ir, ord, biosynth*)

1-Phenyl-1,3,5-hexatriyne P-80105

1,3,5-Hexatriynylbenzene, 9CI

[17814-74-3]

$PhC{\equiv}CC{\equiv}CC{\equiv}CH$

$C_{12}H_6$ M 150.179

Oil. Unstable, prepd. in soln.

▷ Explosive.

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 2586 (*synth, ir, uv*)
Eastmond, R. *et al*, *Tetrahedron*, 1972, **28**, 4591 (*synth*)
Vereshchapin, L.I. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1976, **12**, 1174 (*synth, ir, haz*)
Shim, S.C. *et al*, *J. Org. Chem.*, 1988, **53**, 2410 (*synth*)

1-Phenyl-1-octene, 8CI P-80106

1-Octenylbenzene, 9CI

$PhCH{=}CH(CH_2)_5CH_3$

$C_{14}H_{20}$ M 188.312

(E-)-form [28665-60-3]

Oil. Bp_4 91-94°.

(Z-)-form [42036-72-6]

Oil.

Yamane, T. *et al*, *Tetrahedron*, 1973, **29**, 955 (*synth, ir, pmr*)
Kikukawa, K. *et al*, *J. Org. Chem.*, 1981, **46**, 4885; 1985, **50**, 299 (*synth*)
Lebedev, S.A. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1985, **21**, 652 (*synth, pmr*)

1-Phenyl-2-octene, 8CI P-80107

2-Octenylbenzene, 9CI

$PhCH_2CH{=}CH(CH_2)_4CH_3$

$C_{14}H_{20}$ M 188.312

(E-)-form [42079-83-4]

Oil.

Yamane, T. *et al*, *Tetrahedron*, 1973, **29**, 955 (*synth, ir, pmr*)
Kikukawa, K. *et al*, *J. Org. Chem.*, 1981, **46**, 4885; 1985, **50**, 299 (*synth*)

2-Phenyl-1-octene, 8CI P-80108

(1-Methyleneheptyl)benzene, 9CI. 1-(Hexylethenyl)benzene

[5698-49-7]

$H_2C{=}CPh(CH_2)_5CH_3$

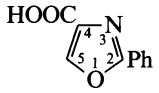
$C_{14}H_{20}$ M 188.312

Oil. Bp_{15} 118°.

Hayashi, T. *et al*, *Tetrahedron Lett.*, 1980, **21**, 3915 (*synth*)
Avasthi, K. *et al*, *Tetrahedron Lett.*, 1980, **21**, 945 (*synth*)
Blatter, K. *et al*, *Synthesis*, 1989, 356 (*synth, ir, pmr, cmr*)

2-Phenyl-4-oxazolecarboxylic acid, 9CI **P-80109**

[23012-16-0]



$C_{10}H_7NO_3$ M 189.170
pK_a 3.41 (H_2O, 20°).

Cornforth, J.W., *The Chemistry of Penicillin*, Clarke H.T. *et al*, Eds, Princeton University Press, 1949, 688.
Brown, D.J. *et al*, *J. Chem. Soc. B*, 1969, **3**, 270 (*pmr*)
Ger. Pat., 2 459 380, (1975); *CA*, **83**, 131577e (*synth*)

2-Phenyl-5-oxazolecarboxylic acid, 9CI **P-80110**

[106833-79-8]

$C_{10}H_7NO_3$ M 189.170
Mp 217-218°.

Belen'kii, L.I. *et al*, *Khim. Geterotsikl. Soedin.*, 1986, 826; *Chem. Heterocycl. Compd.* (*Engl. Transl.*), 654.

5-Phenyl-2-oxazolecarboxylic acid, 9CI **P-80111**

[1014-14-8]

$C_{10}H_7NO_3$ M 189.170
Mp 96-98° dec. pK_a -1.87.

Tanaka, C., *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1965, **85**, 186 (*synth*)
Brown, D.J. *et al*, *J. Chem. Soc. B*, 1969, **3**, 270 (*pmr*)
Ger. Pat., 3 530 213, (1986); *CA*, **105**, 52229n (*synth*)

5-Phenyl-4-oxazolecarboxylic acid, 9CI **P-80112**

[99924-18-2]

$C_{10}H_7NO_3$ M 189.170
Mp 163-164°.

Me ester: [38061-18-6].
$C_{11}H_9NO_3$ M 203.197
Cryst. (hexane). Mp 91-93°.

Et ester: [32998-97-3].
$C_{12}H_{11}NO_3$ M 217.224
$Bp_{0.1}$ 132°.

Schollkopf, U. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1971, **10**, 333 (*ester*)
Yasumasa, H. *et al*, *Tetrahedron Lett.*, 1982, **23**, 235 (*ester*)
Moriya, T. *et al*, *J. Med. Chem.*, 1986, **29**, 333 (*synth, ir*)

5-Phenyl-1,3-pentadiyne **P-80113**

2,4-Pentadiynylbenzene, 9CI

[41268-41-1]

$PhCH_2C{\equiv}CC{\equiv}CH$

$C_{11}H_8$ M 140.184
Isol. from roots of *Artemisia dracunculus* and *Chrysanthemum segetum*. Oil. $Bp_{0.001}$ 45-50°. n_D^{22} 1.5726.

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 39; 1963, **96**, 226 (*isol, uv, ir, struct*)
Klein, J. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1973, 599 (*nmr*)
Harada, R. *et al*, *Phytochemistry*, 1982, **21**, 2009 (*isol, ir, uv, nmr*)

1-Phenyl-2,4-pentadiyn-1-one, 9CI **P-80114**

Benzoylbutadiyne. Demethylcapillone. Desmethylcapillone

[29743-36-0]

$PhCOC{\equiv}CC{\equiv}CH$

$C_{11}H_6O$ M 154.168

Isol. from roots of *Chrysanthemum segetum*, *C. coronarium* and *C. foeniculaceum*. Cryst. (pet. ether). Mp 106°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1963, **96**, 226; 1964, **97**, 1179 (*isol, uv, ir, synth*)
Walton, D.R.M. *et al*, *J. Organomet. Chem.*, 1972, **37**, 45 (*synth*)

1-Phenyl-1,2-pentanedione, 9CI, 8CI **P-80115**

[20895-66-3]

$PhCOCOCH_2CH_2CH_3$

$C_{11}H_{12}O_2$ M 176.215
Liq. Bp_3 82-84°, $Bp_{0.05}$ 60-61°. n_D^{25} 1.5206.

Emmons, W.D. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 4415 (*synth*)
Wagner, P.J. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 8125 (*ir, uv, ms*)
De Kimpe, N. *et al*, *J. Org. Chem.*, 1978, **43**, 2933 (*synth*)
Lee, D.G. *et al*, *J. Org. Chem.*, 1979, **44**, 2726 (*synth*)
Ballistrevi, F.P. *et al*, *Tetrahedron Lett.*, 1986, **27**, 5139 (*synth*)

1-Phenyl-1,3-pentanedione, 9CI, 8CI **P-80116**

1-Benzoyl-2-butanone

[5331-64-6]

$PhCOCH_2COCH_2CH_3$

$C_{11}H_{12}O_2$ M 176.215
Liq. Bp_1 92-94°. n_D^{25} 1.5730.

Hauser, C.R. *et al*, *J. Am. Chem. Soc.*, 1944, **66**, 1220 (*synth*)
Schamp, N. *et al*, *Bull. Soc. Chim. Belg.*, 1966, **75**, 539 (*ms*)
Muir, W.M. *et al*, *J. Org. Chem.*, 1966, **31**, 3790 (*synth*)
Bogovac, M. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 4437 (*synth*)
Koshimura, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 632 (*pmr, tautom*)

1-Phenyl-1,4-pentanedione, 9CI, 8CI **P-80117**

4-Benzoyl-2-butanone

[583-05-1]

$PhCOCH_2CH_2COCH_3$

$C_{11}H_{12}O_2$ M 176.215
Liq. Bp_{20} 168-172°, Bp_{12} 158°.

4-Mono-(2,4-dinitrophenylhydrazone): [71094-27-4].
Cryst. ($CHCl_3$). Mp 197-198°.

Nimgirawath, S. *et al*, *Aust. J. Chem.*, 1976, **29**, 339 (*rev, synth, pmr*)
Faragher, R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1979, 249 (*synth, ir, pmr, ms*)
Clark, J.H. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1983, 2253 (*synth, cmr, pmr*)
Degl'Innocenti, A. *et al*, *Gazz. Chim. Ital.*, 1987, **117**, 645 (*synth*)

1-Phenyl-2,4-pentanedione, 9CI, 8CI **P-80118**

[3318-61-4]

$PhCH_2COCH_2COCH_3$

$C_{11}H_{12}O_2$ M 176.215
Liq. Bp_{10} 133-136°.

Cu chelate: Blue-green cryst. (MeOH). Mp 227-229°.

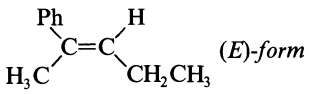
Hauser, C.R. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 6360.
Hampton, K.G. *et al*, *J. Org. Chem.*, 1964, **29**, 3511 (*synth, bibl*)
Org. Synth., 1971, **51**, 128.

2-Phenyl-2-pentene P-80119

Updated Entry replacing P-01445

1-Methyl-1-butenylbenzene, 9CI

[53172-84-2]



(*E*)-*form*

$C_{11}H_{14}$ M 146.232

Bp_{16} 90°.

(***E***)-***form*** [70303-28-5]

Liq. $Bp_{9.5}$ 66-68°.

(***Z***)-***form*** [53172-85-3]

Isol. by glc.

Ando, W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 145 (*synth*)
Zioudrou, C. *et al*, *Tetrahedron*, 1978, **34**, 3181 (*synth, glc, pmr*)
Brown, H.C. *et al*, *J. Org. Chem.*, 1988, **53**, 6009 (*synth, ir, pmr*)

1-Phenyl-2-(phenylthio)ethanone, 9CI P-80120

2-(Phenylthio)acetophenone, 8CI. ω-Phenylmercaptoacetophenone. Phenacyl phenyl sulfide. Benzoyl(phenylthio)methane

[16222-10-9]

$PhCOCH_2SPh$

$C_{14}H_{12}OS$ M 228.314

Needles (EtOH). Mp 53-54°.

Phenylhydrazone: Orange needles (MeOH). Mp 116°.

2,4-Dinitrophenylhydrazone: Bright-red needles (EtOH/EtOAc). Mp 150-150.5°.

S-*Oxide:* [6099-23-6]. *1-Phenyl-2-(phenylsulfinyl)ethanone, 9CI. 2-(Phenylsulfinyl)acetophenone, 8CI. Phenacyl phenyl sulfoxide*

$C_{14}H_{12}O_2S$ M 244.314

Cryst. (C_6H_6/heptane). Mp 79-80°.

S-*Dioxide:* [3406-03-9]. *1-Phenyl-2-(phenylsulfonyl)ethanone, 9CI. 2-(Phenylsulfonyl)acetophenone, 8CI. Phenacyl phenyl sulfone*

$C_{14}H_{12}O_3S$ M 260.313

Cryst. Mp 96°.

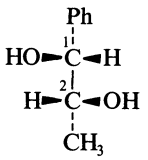
Tröger, J. *et al*, *J. Prakt. Chem.*, 1913, **287**, 289 (*dioxide*)
Kroehnke, F. *et al*, *J. Prakt. Chem.*, 1960, **11**, 256 (*synth*)
Kenny, W.J. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 4019 (*synth, oxide*)
Griesbaum, K. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 1969 (*ir, pmr, oxide, dioxide*)
Krawiec, M. *et al*, *Acta Crystallogr., Sect. C*, 1989, **45**, 354 (*dioxide, cryst struct*)

1-Phenyl-1,2-propanediol, 9CI P-80121

Updated Entry replacing P-01494

1-Phenylpropylene glycol

[1855-09-0]



(1*R*,2*R*)-*form*
Absolute configuration

$C_9H_{12}O_2$ M 152.193

(***1R,2R***)-***form*** [40421-51-0]

D-threo-*form*

Cryst. (pet. ether). Mp 62° (51-53°). $[\alpha]_D^{22}$ −61.5° (c, 4.3 in $CHCl_3$).

Dibenzoyl:

$C_{23}H_{20}O_4$ M 360.409

Needles. Mp 101° (89.5-91°). $[\alpha]_D$ + 0°.

(***1R,2S***)-***form***

Oil. $[\alpha]_D^{21}$ −38.6° (c, 3.2 in $CHCl_3$).

(***1S,2R***)-***form*** [40421-52-1]

D-erythro-*form*

Dibenzoyl: [66841-45-0].

Mp 95-97°. $[\alpha]_D$ −60.9° (c, 0.46 in $CHCl_3$).

(***1RS,2RS***)-***form*** [1075-05-4]

(±)-threo-*form*

Cryst. (pet. ether). Mp 52-54°.

Di-Ac: [21145-70-0].

$C_{13}H_{16}O_4$ M 236.267

Bp_1 106-112°.

Dibenzoyl: [21759-66-0].

Mp 96-97°.

(***1RS,2SR***)-***form*** [1075-04-3]

(±)-erythro-*form*

Powder (C_6H_6/pet. ether). Mp 91-92.5° (89-91°).

Di-Ac: [21145-69-7].

$Bp_{0.4}$ 109°.

Dibenzoyl: [21759-65-9].

Cryst. (MeOH). Mp 96-97°.

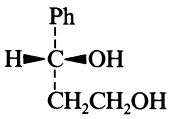
[1075-05-4, 40560-98-3, 54826-39-0]

Witkop, B. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 197 (*abs config*)
Bowlus, S.B. *et al*, *J. Org. Chem.*, 1974, **39**, 3309 (*synth*)
Cowles, C.R. *et al*, *J. Org. Chem.*, 1975, **40**, 1302 (*synth, pmr*)
Fuganti, C. *et al*, *Chem. Ind. (London)*, 1977, 983 (*synth*)
Chrysochou, P. *et al*, *Tetrahedron*, 1977, **33**, 2103 (*synth*)
Zioudrou, C. *et al*, *Tetrahedron*, 1977, **33**, 2103 (*synth*)
Imuta, M. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 3990 (*synth*)
Takeshita, M. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1085 (*synth, bibl*)

1-Phenyl-1,3-propanediol, 9CI P-80122

Updated Entry replacing P-01495

[4850-49-1]



(*R*)-*form*

$C_9H_{12}O_2$ M 152.193

R-form [103548-16-9]

Oil.

3-O-*Methanesulfonyl:* [115290-78-3].

Oil.

(±)-***form***

Oil. Bp_2 126°.

Dibenzoyl:

$C_{23}H_{20}O_4$ M 360.409

Needles (ligroin). Mp 51°.

Bis-4-nitrobenzoyl: Mp 110-110.5°.

Di-Me ether: [26278-67-1]. *1,3-Dimethoxy-1-phenylpropane*

$C_{11}H_{16}O_2$ M 180.246

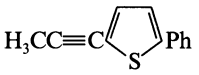
Bp 215-217° part. dec. , Bp_{15} 94-95°.

[96854-34-1, 115290-77-2]

Searles, S. *et al*, *J. Org. Chem.*, 1959, **24**, 1770 (*synth*)
Schaal, C., *Bull. Soc. Chim. Fr.*, 1973, 3083 (*synth*)
Gao, Y. *et al*, *J. Org. Chem.*, 1988, **53**, 4081 (*synth, pmr*)

2-Phenyl-5-(1-propynyl)thiophene, 8CI **P-80123**

[1204-82-6]



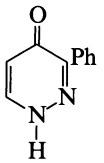
$C_{13}H_{10}S$ M 198.288

Isol. from leaf oil of *Coreopsis grandiflora* and from *C. lanceolata*. Shows nematocidal and insecticidal props. Prismatic needles (C_6H_6/pet. ether). Mp 44°.

Sörensen, J.S. *et al*, *Acta Chem. Scand.*, 1958, **12**, 771 (*isol, struct*)
Cymerman-Craig, J. *et al*, *J. Chem. Soc.*, 1963, 3907 (*synth*)
Atkinson, R. *et al*, *J. Chem. Soc. C*, 1967, 578 (*synth, pmr*)
Nakajima, S. *et al*, *Agric. Biol. Chem.*, 1980, **44**, 1529.
Carpita, A. *et al*, *Tetrahedron*, 1985, **41**, 621 (*synth*)

3-Phenyl-4(1*H*)-pyridazinone, 9CI **P-80124**

[71109-29-0]



$C_{10}H_8N_2O$ M 172.186

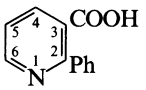
Mp 198-200°.

Gompper, R. *et al*, *Synthesis*, 1979, 385 (*synth, ir, pmr*)

2-Phenyl-3-pyridinecarboxylic acid, 9CI **P-80125**

2-Phenylnicotinic acid, 8CI

[33421-39-5]



$C_{12}H_9NO_2$ M 199.209

Cryst. (Et_2O). Mp 166-168°.

Abramovitch, R.A. *et al*, *Can. J. Chem.*, 1960, **38**, 761 (*synth*)
DuPriest, M.T. *et al*, *J. Org. Chem.*, 1986, **51**, 2021 (*synth, ir, pmr*)

2-Phenyl-4-pyridinecarboxylic acid, 9CI **P-80126**

2-Phenylisonicotinic acid

[55240-51-2]

$C_{12}H_9NO_2$ M 199.209

Mp 268-269°.

Usui, Y. *et al*, *Heterocycles*, 1975, **3**, 155 (*synth, pmr*)

4-Phenyl-2-pyridinecarboxylic acid, 9CI **P-80127**

4-Phenylpicolinic acid

[52565-56-7]

$C_{12}H_9NO_2$ M 199.209

Mp 154-155°.

Takahashi, K. *et al*, *J. Heterocycl. Chem.*, 1978, **15**, 893 (*synth, ir*)

5-Phenyl-2-pyridinecarboxylic acid, 9CI **P-80128**

5-Phenylpicolinic acid

[75754-04-0]

$C_{12}H_9NO_2$ M 199.209

Cryst. (pet. ether). Mp 156-157°.

Farley, C.P. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 3477 (*synth*)

5-Phenyl-3-pyridinecarboxylic acid, 9CI **P-80129**

5-Phenylnicotinic acid

[10177-12-5]

$C_{12}H_9NO_2$ M 199.209

Cryst. (EtOH). Mp 267-269° (260-263°).

Me ester: [10177-13-6].
$C_{13}H_{11}NO_2$ M 213.235
Mp 48°. $Bp_{0.01}$ 108-115°.

Amide:
$C_{12}H_{10}N_2O$ M 198.224
Mp 177-178°.

Amide;B,HCl: Mp 220-224°.

Dimethylamide:
$C_{14}H_{14}N_2O$ M 226.277
Mp 84°. $Bp_{0.01}$ 160-170°.

Dimethylamide;B,HCl: Mp 187-190°.

Diethylamide: [10211-39-9].
$C_{16}H_{18}N_2O$ M 254.331
CNS depressant; lysergic acid analogue. Mp 82°. $Bp_{0.04}$ 146-151°.

Diethylamide;B,HCl: Mp 152-155°.

Farley, C.P. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 3477 (*synth*)
Julia, M. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2387 (*synth, derivs, uv*)
Johnson, F.A. *et al*, *J. Pharm. Sci.*, 1973, **62**, 1881 (*synth, derivs*)

4-Phenyl-2,6-pyridinedicarboxylic acid, 9CI **P-80130**

[83463-12-1]

$C_{13}H_9NO_4$ M 243.218

Cryst. + $2.5H_2O$. Mp 218-220° dec.

Di-Me ester: [117095-81-5].
$C_{15}H_{13}NO_4$ M 271.272
Mp 149-150°.

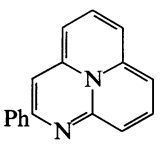
Di-Et ester: [117095-82-6].
$C_{17}H_{17}NO_4$ M 299.326
Cryst. Mp 118-120°.

van Staveren, C.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 8134 (*synth, pmr, cmr*)

2-Phenylpyrimido[2,1,6-*de*]quinolizine, 9CI **P-80131**

2-Phenyl-1,9b-diazaphenalene. 2-Phenyl-1-azacycl[3.3.3]azine

[121902-49-6]



$C_{17}H_{12}N_2$ M 244.295

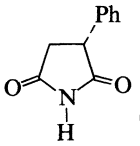
Unstable greenish-brown ppt.

B,HBr: Mp >300°.

Matsuda, Y. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 4307 (*synth, uv, pmr*)

3-Phenyl-2,5-pyrrolidinedione P-80132

3-Phenylsuccinimide



(*R*)-*form*

▷ WN3325000.

(*R*)-*form*

Mp 83-94°. $[\alpha]_D^{20}$ +151° (c, 2 in EtOH). Not opt. pure.

(±)-*form*

Mp 90°.

N-*Me:* [86-34-0]. *1-Methyl-3-phenyl-2,5-pyrrolidinedione, 9CI. N-Methyl-2-phenylsuccinimide.* ***Phensuximide,*** **BAN, INN.** *Epimid. Lepsol. Lifene. Milontin. Milonton. Mirontin. Petimid. Succitimal. PM 334. Fensuximide*

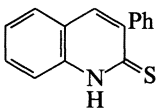
$C_{11}H_{11}NO_2$ M 189.213

Anticonvulsant. Fine cryst. (EtOH). Mp 71-73°.

Wegschieder, R. *et al, Monatsh. Chem.*, 1903, **24**, 422 (*synth*)
Miller, C.A. *et al, J. Am. Chem. Soc.*, 1951, **73**, 4895 (*synth, pharmacol, deriv*)
Glazko, A.J. *et al, J. Pharmacol. Exp. Ther.*, 1954, **111**, 413 (*pharmacol, deriv*)
Turczan, J.W. *et al, J. Pharm. Sci.*, 1973, **62**, 1705 (*pmr*)
Kracmar, J. *et al, Pharmazie*, 1976, **31**, 363 (*uv*)
Ferrendelli, J.A. *et al, Adv. Neurol.*, 1980, **27**, 587 (*rev, deriv*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press London, 1982, 6618 (*deriv*)
Polonski, T., *J. Chem. Soc., Perkin Trans.* 1, 1988, 629 (*synth, ir, pmr, cd*)

3-Phenyl-2(1*H*)-quinolinethione P-80133

[85274-02-8]



$C_{15}H_{11}NS$ M 237.325

Solid. Mp 242-244°.

Blackburn, T.P. *et al, J. Med. Chem.*, 1987, **30**, 2252 (*synth, pmr*)

2-Phenyl-1-(selenocyanato)acetylene P-80134

Selenocyanic acid phenylethynyl ester, 9CI

[114908-26-8]

$PhC{\equiv}CSeCN$

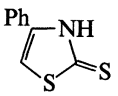
C_9H_5NSe M 206.105

Pale yellow oil.

Meinke, P.T. *et al, J. Org. Chem.*, 1988, **53**, 3632 (*synth, pmr, cmr, ir, ms*)

4-Phenyl-2(3*H*)-thiazolethione, 9CI P-80135

[2103-88-0]



$C_9H_7NS_2$ M 193.293

Mp 141°, Mp 173°.

Vernin, G. *et al, Bull. Soc. Chim. Fr.*, 1963, 2498 (*synth*)
Nalini, V. *et al, J. Chem. Soc., Chem. Commun.*, 1987, 1046 (*cryst struct*)

(Phenylthio)acetaldehyde P-80136

[66303-55-7]

$PhSCH_2CHO$

C_8H_8OS M 152.217

Oxime:

C_8H_9NOS M 167.231

Pale-yellow viscous oil.

Di-Et acetal:

$C_{12}H_{18}OS$ M 210.340

Liq. $Bp_{0.8}$ 103-104°.

Kanemasa, S. *et al, Chem. Pharm. Bull.*, 1988, **61**, 3973.

2-(Phenylthio)propene P-80137

[(*1-Methylethenyl*)*thio*]*benzene, 9CI. Isopropenyl phenyl sulfide*

[7594-43-6]

$H_2C{=}C(SPh)CH_3$

Liq. Bp_9 81-86°, $Bp_{0.8}$ 47°.

S-*Dioxide: Isopropenyl phenyl sulfone*

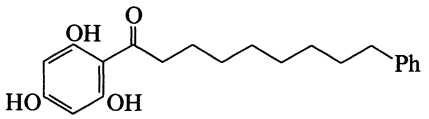
$C_9H_{10}O_2S$ M 182.243

Light-sensitive oil. d^{20} 1.19. $Bp_{4.5}$ 142°.

Groen, S.H. *et al, J. Org. Chem.*, 1968, **33**, 2218 (*synth, pmr*)
Weringa, W.D., *Tetrahedron Lett.*, 1969, 273 (*ms*)
Parham, W.E. *et al, Bull. Chem. Soc. Jpn.*, 1972, **45**, 509 (*synth, ir, uv, pmr*)
Groebel, B.T. *et al, Chem. Ber.*, 1977, **110**, 867 (*synth, pmr, ir*)
Reich, H.J. *et al, J. Org. Chem.*, 1981, **46**, 2775 (*synth, pmr*)
Cory, R.M. *et al, J. Org. Chem.*, 1984, **49**, 3898 (*dioxide*)
Fiandanese, V. *et al, Synthesis*, 1987, 1034 (*synth, pmr*)

9-Phenyl-1-(2,4,6-trihydroxyphenyl)-1-nonanone P-80138

[119736-95-7]



$C_{21}H_{26}O_4$ M 342.434

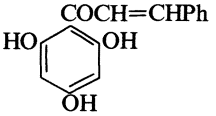
Constit. of *Horsfieldia glabra*. Cryst. (MeOH). Mp 71-72°.

Pinto, M.M.M. *et al, Phytochemistry*, 1988, **27**, 3988.

3-Phenyl-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one P-80139

Updated Entry replacing P-20120

2′,4′,6′-Trihydroxychalcone



$C_{15}H_{12}O_4$ M 256.257

2-Me ether: [18956-16-6]. *1-(2,4-Dihydroxy-6-methoxyphenyl)-3-phenyl-2-propen-1-one, 9CI. 2′,4′-Dihydroxy-6′-methoxychalcone.* ***Cardamonin***

$C_{16}H_{14}O_4$ M 270.284

Isol. from *Boesenbergia pandurata*. Yellow needles ($CHCl_3$/hexane). Mp 199-200°.

4-Me ether: 1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-2-propen-1-one. 2′,6′-Dihydroxy-4′-methoxychalcone

$C_{16}H_{14}O_4$ M 270.284

Isol. from *B. pandurata*. Orange needles ($CHCl_3$/hexane). Mp 163.5-164.5°.

4′-Me ether: [18956-15-5]. *1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-2-propen-1-one. 2′,6′-Dihydroxy-4′-methoxychalcone*
$C_{16}H_{14}O_4$ M 270.284
Constit. of the leaves of *Lindera umbellata*. Red-brown needles. Mp 161-162°.

2′,4′-Di-Me ether: [1775-97-9]. *1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-phenyl-2-propen-1-one. 2′-Hydroxy-4′,6′-dimethoxychalcone*
$C_{17}H_{16}O_4$ M 284.311
Constit. of *Piper methysticum*. Cryst. (MeOH aq.). Mp 91°.

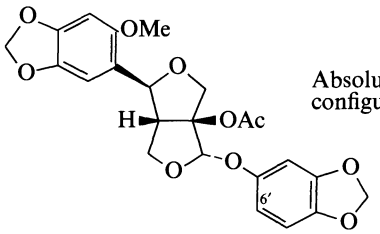
Tri-Me ether: 2′,4′,6′-Trimethoxychalcone
$C_{18}H_{18}O_4$ M 298.338
Yellow needles. Mp 82-84°.

2-Dihydro: see 1-(2,4,6-*Trihydroxyphenyl*)-3-*phenyl*-1-*propanone*, *T*-80332

Haensel, R. *et al*, *Z. Naturforsch.*, *B*, 1963, **18**, 370 (*Flavokawin B*)
Kimura, Y. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1968, **88**, 239 (*isol*)
Hayashi, N. *et al*, *Chem. Ind.* (*London*), 1969, 1779 (*isol*)
Jaipetch, T. *et al*, *Aust. J. Chem.*, 1982, **35**, 351 (*isol*)

Phrymarolin II P-80140

Updated Entry replacing P-60142
1-Acetoxy-6-(2-methoxy-4,5-methylenedioxyphenyl)-2-(3,4-methylenedioxyphenoxy)-3,7-dioxabicyclo[3.3.0]octane
[23720-86-7]



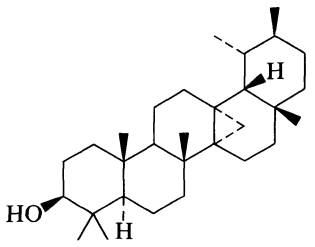
$C_{23}H_{22}O_{10}$ M 458.421
Isol. from root of *Phyrma leptostachya*. Cryst. (Et_2O and EtOAc). Mp 161-162°. $[\alpha]_D$ +117.6° (c, 2.72 in dioxan).

6′-Methoxy: [38303-95-6]. ***Phrymarolin I***
$C_{24}H_{24}O_{11}$ M 488.447
From *P. leptostachya*. Cryst. Mp 155-157°. $[\alpha]_D$ +131.3° (dioxan).

Taniguchi, E. *et al*, *Agric. Biol. Chem.*, 1969, **33**, 466; 1972, **36**, 1489 (*isol*)
Ishibachi, F. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 4361 (*synth, abs config*)

Phyllanthol P-80141

13,27-Cycloursan-3β-ol, 9CI
[546-51-0]

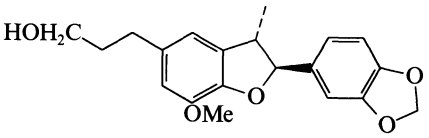


$C_{30}H_{50}O$ M 426.724

Isol. from *Phyllanthus engleri*. Needles ($CHCl_3$/pet. ether). Mp 233-234°. $[\alpha]_D^{15}$ +43° ($CHCl_3$).

Cole, A.R.H., *J. Chem. Soc.*, 1954, 3810 (*struct*)
Sengupta, P. *et al*, *Phytochemistry*, 1966, **5**, 531 (*isol*)

Phyllnirurin P-80142

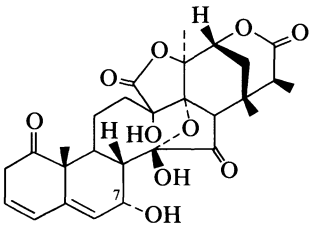


$C_{20}H_{22}O_5$ M 342.391
Constit. of *Phyllanthus niruri*.

Singh, B. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 48 (*isol, ir, pmr*)

Physalin L P-80143

Updated Entry replacing P-60147
[113146-74-0]



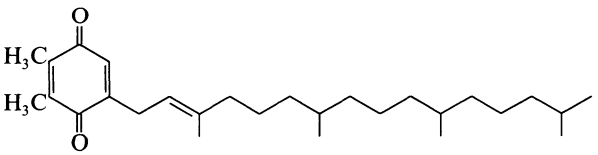
$C_{28}H_{32}O_{10}$ M 528.555
Constit. of *Physalis alkekengi*. Cryst. (2-propanol). Mp 248-249°. $[\alpha]_D^{24}$ −118° (c, 0.3 in Me_2CO).

7-Deoxy: [117591-92-1]. ***Physalin M***
$C_{28}H_{32}O_9$ M 512.555
Constit. of *P. alkekengi*. Cryst. (2-propanol). Mp 224-227°. $[\alpha]_D^{24}$ −106° (c, 0.34 in Me_2CO).

Kawai, M. *et al*, *Phytochemistry*, 1987, **26**, 3313 (*Physalin L*)
Kawai, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 2696 (*Physalin M*)

Phytylplastoquinone P-80144

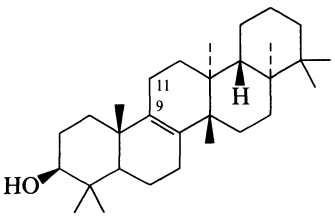
[1177-24-8]



$C_{28}H_{46}O_2$ M 414.670
Isol. from two strains of *Euglena gracilis*. Oil. λ_{max} 254, 261 nm (hexane).

Whistance, G.R. *et al*, *Phytochemistry*, 1970, **9**, 213.

Pichierenol P-80145



$C_{30}H_{50}O$ M 426.724
Ac: ***Pichierenyl acetate***

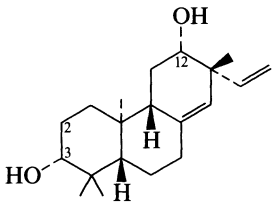
$C_{32}H_{52}O_2$ M 468.762
Constit. of roots of *Picris hieracioides*. Cryst. Mp 272.5-273.5°. $[\alpha]_D^{23}$ −31.2° (c, 0.3 in $CHCl_3$).

$\Delta^{9(11)}$-*Isomer, Ac:* ***Isopichierenyl acetate***
$C_{32}H_{52}O_2$ M 468.762
Constit. of *P. hieracioides*. Cryst. Mp 248.5-249.5°. $[\alpha]_D^{23}$ −2.6° (c, 0.1 in $CHCl_3$).

Shiojima, K. *et al*, *Tetrahedron Lett.*, 1989, **30**, 6873.

ent-8(14),15-Pimaradiene-3β,12β-diol P-80146

Yucalexin P-21



$C_{20}H_{32}O_2$ M 304.472
Constit. of cassava roots (*Manihot esculenta*).

3-Ketone: [119626-50-5]. ent-12β-*Hydroxy*-8(14),15-*pimaradien*-3-*one*. ***Yucalexin P-13***
$C_{20}H_{30}O_2$ M 302.456
Constit. of *M. esculenta*.

12-Ketone: [119626-49-2]. ent-3β-*Hydroxy*-8(14),15-*pimaradien*-12-*one*. *Yucalexin P*-12
$C_{20}H_{30}O_2$ M 302.456
Constit. of *M. esculenta*.

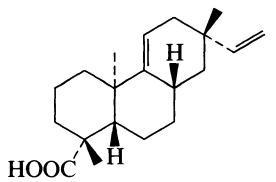
3,12-Diketone: [95523-20-9]. ent-8(14),15-*Pimaradiene*-3,12-*dione*. ***Yucalexin P-4***
$C_{20}H_{28}O_2$ M 300.440
Constit. of *M. esculenta*.

2-Oxo: [119642-82-9]. ent-3β,12β-*Dihydroxy*-8(14),15-*pimaradien*-2-*one*. ***Yucalexin P-17***
$C_{20}H_{30}O_3$ M 318.455
Constit. of *M. esculenta*.

Sakai, T. *et al*, *Phytochemistry*, 1988, **27**, 3769.

ent-9(11),15-Pimaradien-19-oic acid P-80147

[119290-87-8]



$C_{20}H_{30}O_2$ M 302.456
Constit. of *Acanthopanax koreanum*. Amorph. powder. Mp 135-136°.

Kim, Y.H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1080.

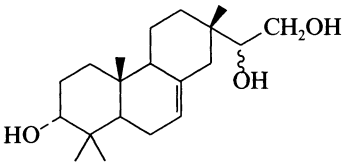
ent-9,(11),15-Pimaradien-19-ol P-80148

$C_{20}H_{32}O$ M 288.472
Constit. of *Acanthopanax koreanum*. Needles (hexane). Mp 73-74°. $[\alpha]_D^{25}$ −14.94° (c, 0.19 in $CHCl_3$).

Ac: 19-Acetoxy-9,(11),15-pimaradiene
$C_{22}H_{34}O_2$ M 330.509
Constit. of *A. koreanum*. Oil. $[\alpha]_D^{25}$ −8.82° (c, 0.34 in $CHCl_3$).

Kim, Y.H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1080 (*isol, pmr, cmr*)

7-Pimarene-3,15,16-triol P-80149



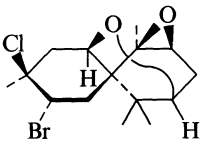
$C_{20}H_{36}O_3$ M 324.503

3α-form
Constit. of *Agathis vitiensis*. Needles (EtOAc). Mp 170-175°. $[\alpha]_D^{17}$ −22° (c, 1 in MeOH).

Cambie, R.C. *et al*, *Phytochemistry*, 1989, **28**, 1675.

Pinnatazone P-80150

[119765-94-5]

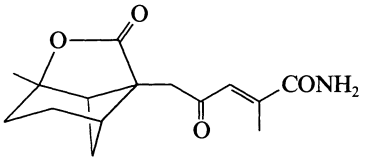


$C_{15}H_{22}BrClO_2$ M 349.694
Constit. of *Laurencia pinnatifida*. Cryst. (MeOH). Mp 190-192°. $[\alpha]_D$ +4.34° (c, 0.23 in $CHCl_3$).

Atta-ur-Rahman, *et al*, *Phytochemistry*, 1988, **27**, 3879 (*isol, cryst struct*)

Pinthuamide P-80151

[122279-83-8]

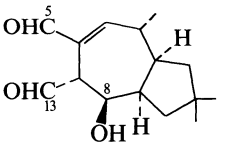


$C_{15}H_{19}NO_4$ M 277.319
Metab. of fungus *Ampulliferina* sp. Needles (EtOAc). Mp 190-193°. $[\alpha]_D^{20}$ +73.4° (c, 1.0 in EtOH).

Kimura, Y. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1267 (*cryst struct*)

Piperdial P-80152

[100288-36-6]



$C_{15}H_{22}O_3$ M 250.337
Constit. of *Lactarius necator*. $[\alpha]_D^{23}$ +77° (c, 0.8 in Et_2O).

13-Alcohol: [100288-35-5]. ***Piperalol***
$C_{15}H_{24}O_3$ M 252.353
Constit. of *L. necator*. $[\alpha]_D^{23}$ +57° (c, 4.3 in Et_2O).

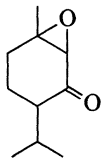
5,13-Bisalcohol, 8-epimer: [118918-26-6]. ***8-Epipertriol***
$C_{15}H_{26}O_3$ M 254.369
Constit. of *L. necator*. Cryst. Mp 108-114°. $[\alpha]_D^{20}$ −36.6° (c, 1 in $CHCl_3$).

Sterner, O. *et al*, *Tetrahedron Lett.*, 1985, **26**, 3163 (*isol, struct*)
Daniewski, W.M. *et al*, *Phytochemistry*, 1988, **27**, 3315 (*isol, deriv*)

Piperitone oxide P-80153

*6-Methyl-3-(1-methylethyl)-7-oxabicyclo[4.1.0]heptan-2-one, 9CI. 1,2-Epoxy-*p*-menthan-3-one, 8CI. 2,3-Epoxy-6-isopropyl-3-methylcyclohexanone*

[5286-38-4]



$C_{10}H_{16}O_2$ M 168.235

Stereochem. not clear. Isol. from *Mentha sylvestris* oil and other essential oils. Cryst. (hexane). d_{25}^{25} 1.01. Mp 14.5-15.5°. $[\alpha]_D^{22}$ −177.0° (c, 0.96 in EtOH). n_D^{20} 1.4624. Poss. identical with Dihydrolippione.

Semicarbazone: Cryst. Mp 199-200°. $[\alpha]_{25}$ +213° (c, 0.29 in 95% EtOH aq.).

2,4-Dinitrophenylhydrazone: Cryst. Mp 115-117°.

[4713-37-5, 4713-38-6, 20303-83-7, 57130-28-6, 103476-50-2]

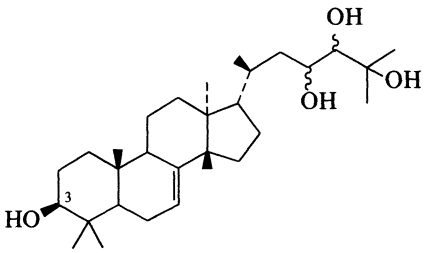
Reitsema, R.H. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 3792 (*isol*)
Nigam, I.C. *et al*, *Can. J. Chem.*, 1963, **41**, 1535 (*occur*)
Klein, E. *et al*, *Tetrahedron*, 1963, **19**, 1091 (*synth*)
Gacs-Baitz, E. *et al*, *Org. Magn. Reson.*, 1984, **22**, 738 (*pmr, cmr*)

Piscidinol B P-80154

Updated Entry replacing P-50204

7-Tirucallene-3β,23ξ,24ξ,25-tetrol

[100295-68-9]



$C_{30}H_{52}O_4$ M 476.738

Constit. of *Walsura piscidia*. Cryst. (MeOH). Mp 240°.

3-Ketone: [100198-09-2]. *23ξ,24ξ,25-Trihydroxy-7-tirucallen-3-one.* ***Piscidinol A***

$C_{30}H_{50}O_4$ M 474.723

From *W. piscidia*, also from *Phellodendron chinense* and *Turrea nilotica*. Cryst. (MeOH). Mp 195°. $[\alpha]_D^{25}$ −90° (c, 1 in $CHCl_3$). The isolate from *T. nilotica* (amorph., no further details) could be a stereoisomer.

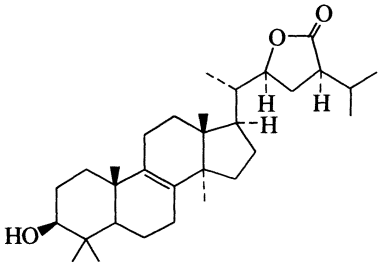
[115404-56-3]

Purushothaman, K.K. *et al*, *Phytochemistry*, 1985, **24**, 2349 (*isol*)
Mulholland, D.A. *et al*, *Phytochemistry*, 1988, **27**, 1220, 1809 (*isol, deriv*)
Kaur, K.J. *et al*, *Phytochemistry*, 1988, **27**, 1809 (*isol, deriv*)

Pisolactone P-80155

Updated Entry replacing P-20140

[87164-33-8]



$C_{31}H_{50}O_3$ M 470.734

Constit. of fungus *Pisolithus tinctorius*. Prisms (MeOH). Mp 279-280°. $[\alpha]_D^{28}$ +60° (c, 1 in $CHCl_3$).

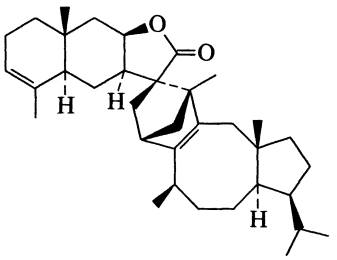
3-Ketone: [119539-75-2]. ***3-Oxopisolactone***

$C_{31}H_{48}O_3$ M 468.718

Metab. of *P. tinctorius*. Cryst. (MeOH). Mp 248-250°. $[\alpha]_D$ +79° (c, 1.4 in $CHCl_3$).

Lobo, A.M. *et al*, *Tetrahedron Lett.*, 1983, **24**, 2205 (*isol, cryst struct*)
Lobo, A.M. *et al*, *Phytochemistry*, 1988, **27**, 3569 (*deriv*)

Plagiospirolide A P-80156

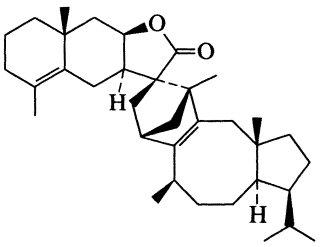


$C_{35}H_{52}O_2$ M 504.795

Constit. of liverwort *Plagiochila moritziana*. Needles (hexane). Mp 196-198°. $[\alpha]_D^{20}$ +411.9° (c, 0.36 in $CHCl_3$).

Spörle, J. *et al*, *Tetrahedron*, 1989, **45**, 5003 (*cryst struct*)

Plagiospirolide B P-80157



$C_{35}H_{52}O_2$ M 504.795

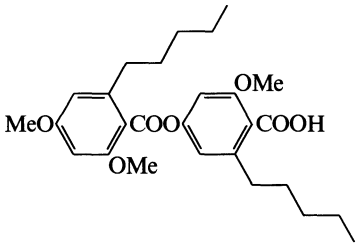
Constit. of liverwort *Plagiochila moritziana*. Oil. $[\alpha]_D^{20}$ +59.2° (c, 1.176 in $CHCl_3$).

Spörle, H. *et al*, *Tetrahedron*, 1989, **45**, 5003.

Planaic acid P-80158

4-Carboxy-3-methoxy-5-pentylphenyl 2,4-dimethoxy-6-pentylbenzoate, 9CI. 4-Hydroxy-6-pentyl-o-anisic acid 2,4-dimethoxy-6-pentylbenzoate, 8CI

[5366-07-4]



$C_{27}H_{36}O_7$ M 472.577

Isol. from *Lecidea plana* and *L. lithophila*. Needles (MeOH). Mp 110-111°.

Huneck, S. *et al*, *Z. Naturforsch.*, *B*, 1965, **20**, 1119, 1137 (*isol, ir, pmr, struct*)
Huneck, S. *et al*, *Tetrahedron*, 1968, **24**, 2707 (*ms*)
Elix, J.A., *Aust. J. Chem.*, 1974, **27**, 1767 (*synth, pmr, ms*)

Plastoquinone 4 P-80159

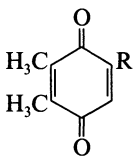
Plastoquinone 20

$C_{28}H_{40}O_2$ M 408.623

Isol. from leaves of *Aesculus hippocastanum*. Unstable orange oil.

Eck, H. *et al*, *Z. Naturforsch.*, *B*, 1963, **18**, 446 (*isol, uv, ir, pmr*)
Das, B.C. *et al*, *Biochem. Biophys. Res. Commun.*, 1965, **21**, 318 (*uv*)
Misiti, D. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 1407 (*struct*)

Plastoquinones P-80160

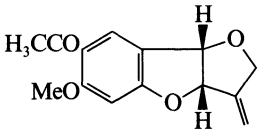


A family of 2,3-dimethyl-5-polyprenyl-1,4-benzoquinones found in plant tissues. R represents a prenyl side-chain which may be unsubstituted (Plastoquinones), monohydroxylated (Plastoquinone C), monoacylated (Plastoquinone B), or monohydroxylated and monoacylated (Plastoquinone Z).The latter classes appear to be confined to higher plant tissues.

Whistance, G.R. *et al*, *Phytochemistry*, 1970, **9**, 213 (*isol*)
Pennock, J.F., *Biochem. Soc. Trans.*, 1983, **11**, 504 (*rev, biosynth*)

Platypodantherone P-80161

[118855-44-0]



$C_{14}H_{14}O_4$ M 246.262

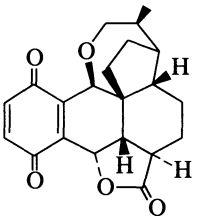
Constit. of *Platypodanthera melissaefolia*. Oil.

Paredes, L. *et al*, *Phytochemistry*, 1988, **27**, 3329.

Pleurotin P-80162

Geogenine

[1404-23-5]



$C_{21}H_{22}O_5$ M 354.402

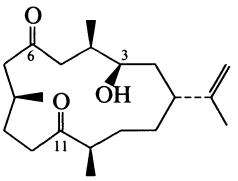
Benzoquinone antibiotic. Identity of Pleurotin and Geogenine not fully established. Isol. from *Pleurotus griseus*, *Geopetalum geogerium* and *Hohenbuehalia geogenius*. Active against gram-positive bacteria, mycobacteria and possesses antitumour activity. Amber cryst. Mp 200-215° dec. $[\alpha]_D^{23}$ −20° ($CHCl_3$).

[77550-91-5]

Robbins, W.J. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1947, **33**, 171 (*isol*)
Arigoni, D., *Pure Appl. Chem.*, 1968, **17**, 331 (*struct*)
Grandjean, J. *et al*, *Tetrahedron Lett.*, 1974, 1893 (*pmr, cmr, struct*)
Fr. Pat., 2 407 718, (1979); *CA*, **91**, 173367 (*isol*)
Riondel, J. *et al*, *Acta Crystallogr.*, *Sect. C*, 1981, **37**, 1309 (*cryst struct*)
Riondel, J. *et al*, *Arzneim.-Forsch.*, 1981, **31**, 293 (*isol, uv, ir, pmr, cmr, ms*)

Plexaurolone P-80163

[75248-46-3]



$C_{20}H_{34}O_3$ M 322.487

Metab. of *Plexaura* sp. Cryst. (Me_2CO/pet. ether). Mp 110-111°.

*11*R*-Alcohol:* [119979-75-8]. ***Dihydroplexaurolone***
$C_{20}H_{36}O_3$ M 324.503
Metab. of *P.* sp. Prisms (Me_2CO/hexane). Mp 125-126°. $[\alpha]_D$ +42° (c, 0.12 in $CHCl_3$).

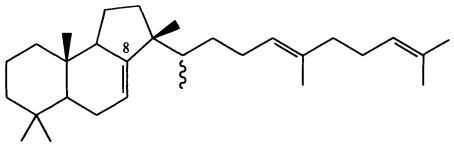
3-Ketone: [119979-76-9]. ***Dehydroplexaurolone***
$C_{20}H_{32}O_3$ M 320.471
Metab. of *P.* sp. Needles (Me_2CO/pet. ether). Mp 93-95°. $[\alpha]_D$ +48° (c, 0.27 in $CHCl_3$).

3-Ketone, stereoisomer: [120053-65-8]. ***Isodehydroplexaurolone***
$C_{20}H_{32}O_3$ M 320.471

Metab. of *P.* sp. Cubes (Me_2CO/pet. ether). Mp 196-199°. $[\alpha]_D$ −11° (c, 0.09 in $CHCl_3$). Stereoisomeric at C-4 and/or C-12.

Ealick, S.E. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1901 (*cryst struct*)
Chan, W.R. *et al*, *Tetrahedron*, 1989, **45**, 103 (*cryst struct*)

7,17,21-Podiodatriene P-80164



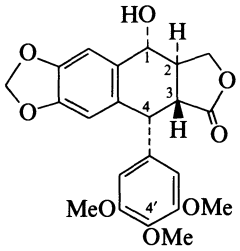
$C_{30}H_{50}$ M 410.725
Constit. of rhizomes of *Polypodioides niponica*. Oil. $[\alpha]_D^{23}$ −11.5° (c, 0.2 in $CHCl_3$).

Δ^8-*Isomer:* ***8,17,21-Podiodatriene***
Constit. of *P. niponica*. Oil. $[\alpha]_D^{23}$ +11.7° (c, 0.2 in $CHCl_3$).

Arai, Y. *et al*, *Tetrahedron Lett.*, 1989, **30**, 7209.

Podophyllotoxin P-80165

Updated Entry replacing P-50227
[518-28-5]



$C_{22}H_{22}O_8$ M 414.411
Lignan from *Podophyllum emodi* rhizomes. Also isol. from *P. peltatum*, other *P.* spp., *Diphylleia grayi*, *Callitris drummondii* and *Juniperus* spp. Potent cytotoxin. Cell division inhibitor. Cryst. (Me_2CO aq. or MeOH). Mp 117-118°. $[\alpha]_D^{14}$ −101.3° (EtOH). 4 Crystal modifications reported. Mp's up to 188-189° have been reported for carefully dried samples.

▷ Highly toxic orally, exp. carcinogen.

Ac: [1180-34-3].
Cryst. (MeOH). Mp 209.5-210.5°. $[\alpha]_D^{20}$ −143° (c, 1.0 in $CHCl_3$).

1-β-D-Glucoside:
$C_{28}H_{32}O_{13}$ M 576.553
Isol. from *P. emodi*. Amorph. solid. Mp 149-152°. $[\alpha]_D^{20}$ −65° (c, 0.5 in H_2O), $[\alpha]_D$ −75° (c, 0.6 in MeOH), $[\alpha]_D$ −117° (c, 0.67 in Py).

1-Epimer: [4375-07-9]. *Epipodophyllotoxin*
Needles (EtOH aq.). Mp 159.4-161.2°. $[\alpha]_D^{20}$ −75° (c, 1 in $CHCl_3$).
▷ LV2520000.

3-Epimer: [477-47-4]. ***Picropodophyllin***
$C_{22}H_{22}O_8$ M 414.411
Isol. from *P. emodi*, *Diphylleia grayi* and others. Needles (MeOH or C_6H_6). Mp 226-227°. $[\alpha]_D$ +5.3° ($CHCl_3$).

3-Epimer, O-β-D-Glucopyranoside: Picropodophyllin glucoside
$C_{28}H_{32}O_{13}$ M 576.553
Isol. from *P. emodi*. Needles (H_2O). Mp 237-238°. $[\alpha]_D^{20}$ −11.5° (Py).

4'-O-De-Me: ***4'-Demethylpodophyllotoxin.*** *4'-Desmethylpodophyllotoxin*
$C_{21}H_{20}O_8$ M 400.384
Isol. from *P. emodi*. Prisms or plates (EtOH aq.). Mp 250-251.6°. $[\alpha]_D^{20}$ −130° ($CHCl_3$).

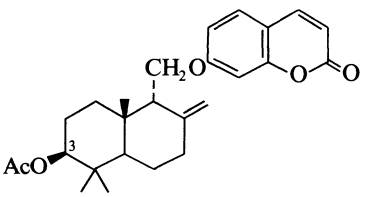
4'-O-De-Me, 1-O-β-D-glucoside:
$C_{27}H_{30}O_{13}$ M 562.526
Isol. from *P. emodi*. Powder. Mp 165-170°. $[\alpha]_D^{20}$ −75° (H_2O).

1,2,3,4-Tetradehydro: ***Dehydropodophyllotoxin***
$C_{22}H_{18}O_8$ M 410.379
Minor constit. of *P. peltatum*. Needles (EtOH). Mp 272-274°. Achiral.

Hartwell, J.L. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 2909 (*isol*)
Nadkarni, M.V. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 1308 (*isol, derivs*)
Kofod, H. *et al*, *Acta Chem. Scand.*, 1954, **8**, 1296 (*Dehydropodophyllotoxin*)
Stoll, A. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 3103 (*Glucosides*)
Schrecker, A.W. *et al*, *J. Org. Chem.*, 1956, **21**, 288, 381 (*props, abs config*)
Gensler, W.J. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 1748 (*synth*)
Gensler, W.J. *et al*, *J. Org. Chem.*, 1966, **31**, 3224 (*synth*)
Duffield, A.M., *J. Heterocycl. Chem.*, 1967, **4**, 16 (*ms*)
Ayres, D.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 1343 (*pmr*)
Petcher, T.J. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1973, 288 (*cryst struct*)
Cannetta, R. *et al*, *Cancer Chemother. Pharmacol.*, 1982, **7**, 103 (*pharmacol*)
Jackson, D.E. *et al*, *Phytochemistry*, 1984, **23**, 1029, 1037 (*biosynth*)
Inamori, Y. *et al*, *Chem. Pharm. Bull.*, 1986, **34**, 3928 (*props*)
Macdonald, D.I. *et al*, *J. Org. Chem.*, 1986, **51**, 4749 (*synth*)
Kamil, W.M. *et al*, *Phytochemistry*, 1986, **25**, 2093 (*biosynth*)
Van der Eycken, J. *et al*, *Tetrahedron*, 1986, **42**, 4297 (*synth*)
Vyas, D.M. *et al*, *Tetrahedron Lett.*, 1986, **27**, 3099 (*synth*)
Jones, D.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1797 (*synth*)
Kaneko, T. *et al*, *Tetrahedron Lett.*, 1987, **28**, 517 (*synth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 919.

Polyanthin P-80166

Updated Entry replacing P-10228
[54631-86-6]



$C_{26}H_{32}O_5$ M 424.536
Isol. from *Ferula polyantha*. Mp 148-149°.

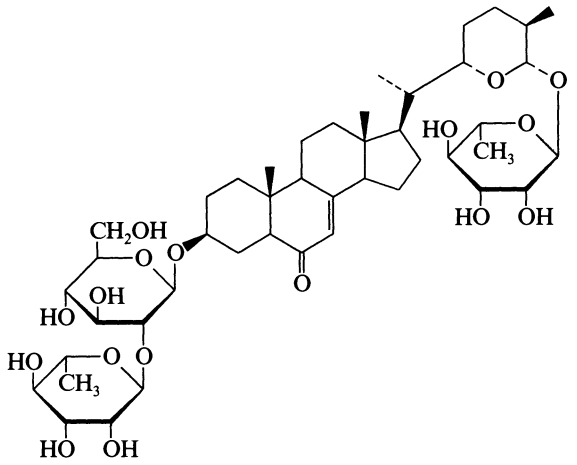
3-Epimer: [54631-85-5]. ***Polyanthinin***
$C_{26}H_{32}O_5$ M 424.536
From *F. polyantha*. Mp 127-129°.

3-Epimer, O-de-Ac: [51819-92-2]. ***Gummosin***
$C_{24}H_{30}O_4$ M 382.499
From *F. gummosa*. Mp 176-177°. $[\alpha]_D$ −54° ($CHCl_3$).

Perel'son, M.E., *Khim. Prir. Soedin.*, 1973, **9**, 490; 1974, **10**, 15; 1975, **11**, 244.
Khasanov, T.Kh. *et al*, *Khim. Prir. Soedin.*, 1974, **10**, 517.

Polypodoside A P-80167

[119784-25-7]



$C_{45}H_{72}O_{17}$ M 885.054

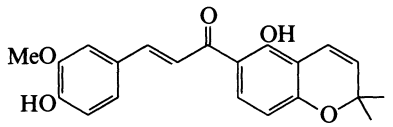
Constit. of rhizomes of *Polypodium glycyrrhiza*. Intensely sweet substance. Needles (EtOH). Mp 198-200°. $[\alpha]_D$ −37° (c, 0.3 in MeOH).

Kim, J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1166 (*isol, pmr, cmr*)

Pongachalcone II P-80168

1-(5-Hydroxy-2,2-dimethyl-2H-1-benzopyran-6-yl)-3-(4-hydroxy-3-methoxyphenyl)-2-propen-1-one, 9CI. 5-Hydroxy-6-(4-hydroxy-3-methoxycinnamoyl)-2,2-dimethyl-2H-1-benzopyran

[64173-09-7]



$C_{21}H_{20}O_5$ M 352.386

Isol. from heartwood of *Pongamia glabra*. Orange-red solid. Mp 175-176° (synthetic).

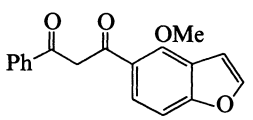
Subrahmanyam, K. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 12 (*isol, struct, synth*)

Pongamol P-80169

Updated Entry replacing P-02168

1-(4-Methoxy-5-benzofuranyl)-3-phenyl-1,3-propanedione, 9CI. 5-Benzoylmethoxy-6-methoxybenzofuran. 5-Benzoylacetyl-4-methoxybenzofuran, 8CI

[484-33-3]



$C_{18}H_{14}O_4$ M 294.306

Isol. from *Pongamia glabra* and *Tephrosia* spp. Used in insecticides and pesticides. Yellow rhombic prisms (EtOH/AcOH). Mp 135-136°. Exists in the enolised form.

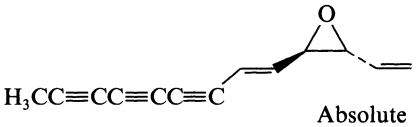
Cu complex: Green rhombohedral tablets ($CHCl_3/Et_2O$). Mp 220-222°.

Rangaswami, S. *et al*, *CA*, 1941, **35**, 5733 (*isol*)
Mukerjee, S.K. *et al*, *J. Chem. Soc.*, 1955, 2048 (*synth*)
Roy, D. *et al*, *Curr. Sci.*, 1977, **46**, 743; *CA*, **88**, 19047 (*isol*)
Sinka, B. *et al*, *Phytochemistry*, 1982, **21**, 1468 (*isol*)
Sighamony, S. *et al*, *Int. Pest Control*, 1983, **25**, 120 (*use*)
Rajain, P. *et al*, *Phytochemistry*, 1988, **27**, 648 (*isol*)
Parmar, V.S. *et al*, *Phytochemistry*, 1989, **28**, 591 (*cryst struct*)

Ponticaepoxide P-80170

2-Ethenyl-3-(1-nonen-3,5,7-triynyl)oxirane, 9CI. 2-(1-Nonen-3,5,7-triynyl)-3-vinyloxirane. 3,4-Epoxy-1,5-tridecadiene-7,9,11-triyne

[3562-36-5]



Absolute configuration

$C_{13}H_{10}O$ M 182.221

(+)-form

Isol. from various Compositae spp., e.g. *Artemisa, Tanacetum, Chrysanthemum, Cladanthus, Achillea* spp. Cryst. (pet. ether). Mp 66°. $[\alpha]_D^{23}$ +201° (c, 1.0 in Me_2CO).

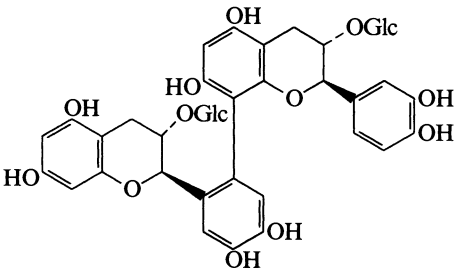
(±)-form

Mp 52°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1960, **93**, 1937; 1962, **95**, 1742; 1964, **97**, 809, 1179; 1966, **99**, 1830 (*isol, uv, struct, abs config*)
Hemmer, E. *et al*, *Acta Chem. Scand.*, 1961, **15**, 691 (*isol*)
Bohlmann, F. *et al*, *Tetrahedron Lett.*, 1965, 1385 (*synth*)

Potentillanin P-80171

[118555-81-0]

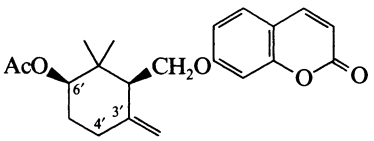


$C_{42}H_{46}O_{22}$ M 902.812

Constit. of *Potentilla viscosa*. Amorph. powder. $[\alpha]_D^{18}$ −80° (c, 1 in Me_2CO aq.).

Zhang, B. *et al*, *Phytochemistry*, 1988, **27**, 3277.

Praealtin A P-80172



$C_{21}H_{24}O_5$ M 356.418

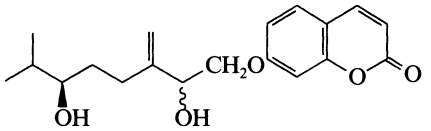
Constit. of *Aster praealtus*. Cryst. (C_6H_6). Mp 163.3°.

$\Delta^{3'4'}$*-Isomer, 6'-de-Ac, 6'-(2-methylbutanoyl):* ***Praealtin B***
$C_{24}H_{30}O_5$ M 398.498
Constit. of *A. praealtus*.

$\Delta^{3'4'}$*Isomer, 6'-de-Ac, 6'-(2-methylbutanoyl):* ***Praealtin C***
$C_{24}H_{30}O_5$ M 398.498
Constit. of *A. praealtus*.

Wilzer, K.A. *et al*, *Phytochemistry*, 1989, **28**, 1729 (*cryst struct, isol*)

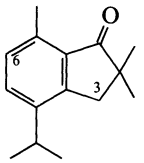
Praealtin D P-80173



$C_{19}H_{24}O_6$ M 348.395
Constit. of *Aster praealtus*. Gum.

Wilzer, K.A. *et al*, *Phytochemistry*, 1989, **28**, 1729.

Primnatrienone P-80174



$C_{15}H_{20}O$ M 216.322

6-Hydroxy: [116173-40-1]. ***6-Hydroxyprimnatrienone***
$C_{15}H_{20}O_2$ M 232.322
Constit. of a *Primnoeides* sp. Cryst. (CH_2Cl_2/hexane). Mp 137-138°.

6-Methoxy: [116173-41-2]. ***6-Methoxyprimnatrienone***
$C_{16}H_{22}O_2$ M 246.349
Constit. of a *P.* sp. Oil.

6-Methoxy, 3-hydroxy: [116173-38-7]. ***3-Hydroxy-6-methoxyprimnatrienone***
$C_{16}H_{22}O_3$ M 262.348
Constit. of *P.* sp. Cryst. (EtOAc/hexane). Mp 122-124°.

6-Methoxy, 3-acetoxy: [116173-39-8]. ***3-Acetoxy-6-methoxyprimnatrienone***
$C_{18}H_{24}O_4$ M 304.385
Constit. of a *P.* sp. Oil. $[\alpha]_D^{20}$ +1.5° (c, 0.3 in $CHCl_3$).

6-Methoxy, 3-oxo: [116173-37-6]. ***6-Methoxy-1,3-primnatrienedione***
$C_{16}H_{20}O_3$ M 260.332
Pale yellow microcryst. Mp 92-93°.

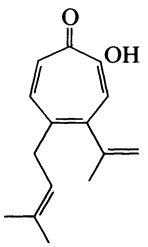
Cambie, R.C. *et al*, *Aust. J. Chem.*, 1988, **41**, 365.

Procerin† P-80175

Updated Entry replacing P-02289

2-Hydroxy-5-(3-methyl-2-butenyl)-4-(1-methylethenyl)-2,4,6-cycloheptatrien-1-one, 9CI. 4-Isopropenyl-5-prenyltropolone. 6-Isopropenyl-5-prenyltropolone

[552-96-5]



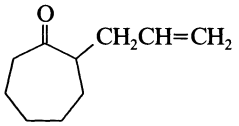
$C_{15}H_{18}O_2$ M 230.306
Present in *Juniperus procera*. Mp 71-72°.

Runeberg, J., *Acta Chem. Scand.*, 1961, **15**, 645 (*ir, synth*)
Kitahara, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1964, **37**, 895 (*synth*)

2-(2-Propenyl)cycloheptanone, 9CI P-80176

2-Allylcycloheptanone

[58105-24-1]



$C_{10}H_{16}O$ M 152.236

(±)-***form*** [115094-62-7]
Liq. with odour of menthol. d_4^{22} 0.93. Bp_{18} 103°.

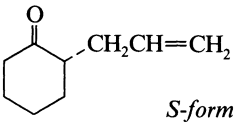
Semicarbazone: Cryst. Mp 145°.

Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1953, 1074 (*synth*)
Dzhemilev, U.M. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1988, 378 (*synth*)

2-(2-Propenyl)cyclohexanone, 9CI P-80177

2-Allylcyclohexanone

[94-66-6]



S-form

C_9H_4O M 128.130

(*S*)-***form*** [36302-35-9]
Bp_{36} 100°. $[\alpha]_D^{23}$ −2.7° (c, 4.11 in $CHCl_3$). Optical purity 20%.

(±)-***form*** [115182-22-4]
Liq. Bp_{12} 79-80°.

Oxime: [59239-07-5].
$C_9H_{15}NO$ M 153.224
Needles. Mp 71°.

2,4-Dinitrophenylhydrazone: Orange needles (EtOH). Mp 149-150°.

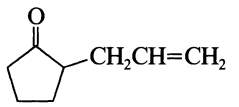
[1044-31-1, 59239-07-5]

Cope, A.C. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 1842 (*synth*)
Optitz, G. *et al*, *Justus Liebigs Ann. Chem.*, 1961, **649**, 47 (*synth, ir*)
Hiroi, K. *et al*, *Chem. Pharm. Bull.*, 1972, **20**, 246 (*synth, cd, ir, ord, abs config*)
Ganem, B., *J. Org. Chem.*, 1975, **40**, 146 (*synth*)
Meyers, A.I. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 3032 (*synth*)
Araujo, H.C. *et al*, *Synthesis*, 1978, **3**, 228 (*synth*)
Murahashi, S.-I. *et al*, *J. Org. Chem.*, 1988, **53**, 4489 (*synth, ir, pmr*)

2-(2-Propenyl)cyclopentanone, 9CI P-80178

2-Allylcyclopentanone

[30079-93-7]



$C_8H_{12}O$ M 124.182

(±)-***form*** [55038-60-3]
Liq. with menthyl odour. 188-190°, Bp_{19} 80°.

Semicarbazone: Cryst. Mp 190° (180°).

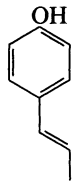
Colonge, J. *et al*, *Bull. Soc. Chim. Fr.*, 1953, 1074 (*synth*)
Lorette, N.B. *et al*, *J. Org. Chem.*, 1961, **26**, 3112 (*synth*)
Oritani, T. *et al*, *Agric. Biol. Chem.*, 1975, **39**, 89 (*synth, ir*)
Dzhemilev, U.M. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1988, 378 (*synth*)
Toru, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4815 (*synth*)

4-(1-Propenyl)phenol, 9CI P-80179

Updated Entry replacing P-30187

1-(4-Hydroxyphenyl)-2-propene. p-Hydroxy-β-methylstyrene. Anol

[539-12-8]



(*E*)-*form*

$C_9H_{10}O$ M 134.177

(*E*)-*form*

Leaflets (H_2O). Mp 93°. Bp_{14} 140°. Dec. on standing in air.

Me ether: [4180-23-8]. *1-Methoxy-4-(1-propenyl)benzene.* ***Anethole.*** *Anistearoptene*

$C_{10}H_{12}O$ M 148.204

Present in anise, fennel and other plant oils. Extensively used in flavour industry. Leaflets (EtOH). Mp 22.5°. Bp 235°.

▷ Mod. toxic. BZ9275000.

3-Methylbutanoyl: Anol isovalerate

$C_{14}H_{18}O_2$ M 218.295

Constit. of *Coreopsis gigantea*. Oil. $Bp_{0.01}$ 60-65° (bath) .

O-(*3-Methyl-2-butenyl*): [78259-41-3]. ***Foeniculin.*** *Feniculin*

$C_{14}H_{18}O$ M 202.296

Isol. from fennel and Chinese star anise oils. Mp 23.5-24.5°.

(*Z*)-*form*

Me ether: [25679-28-1].

Liq. d_4^{20} 0.989. $Bp_{2.5}$ 63-65°. n_D^{20} 1.5550 (93% pure). Low level only permitted in flavours.

[104-46-1]

Späth, E. *et al*, *Ber.*, 1938, **71**, 2708 (*Foeniculin*)
Naves, Y.R., *Helv. Chim. Acta*, 1960, **53**, 230 (*cis*-Anethole)
Briner, E. *et al*, *Helv. Chim. Acta*, 1963, **46**, 2249 (*ir*)
Klamann, D. *et al*, *Chem. Ber.*, 1964, **97**, 2534 (*synth*)
Sørensen, J.S. *et al*, *Acta Chem. Scand.*, 1966, **20**, 992 (*ir*)
Benassi, R. *et al*, *Org. Magn. Reson.*, 1973, **5**, 391 (*pmr*)
Hamacher, H., *Arch. Pharm.* (*Weinheim, Ger.*), 1974, **307**, 309 (*synth*)
Manitto, P. *et al*, *Tetrahedron Lett.*, 1974, 1567 (*biosynth*)
Okely, H.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1981, 897 (*Foeniculin*)
Wenkert, E. *et al*, *Synthesis*, 1983, 701 (*synth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 379.

2-(2-Propenyl)-1,3-propanediol, 9CI P-80180

2-Allyl-1,3-propanediol. 2-Hydroxymethyl-4-penten-1-ol

[42201-43-4]

$H_2C{=}CHCH_2CH(CH_2OH)_2$

$C_6H_{12}O_2$ M 116.160

Liq. Bp_{15} 136-139°, $Bp_{1.0}$ 95-98°.

Kharasch, M.S. *et al*, *J. Org. Chem.*, 1949, **14**, 84 (*synth*)
Wasson, B.K. *et al*, *Can. J. Chem.*, 1961, **39**, 923 (*synth*)
Courtois, G. *et al*, *J. Organomet. Chem.*, 1973, **52**, 241 (*synth, ir, pmr*)
Vite, G.D. *et al*, *J. Org. Chem.*, 1988, **53**, 2555 (*synth*)

3-(1-Propenyl)pyridine, 9CI P-80181

1-(3-Pyridyl)-1-propene

C_8H_9N M 119.166

(*E*)-*form* [52248-76-7]

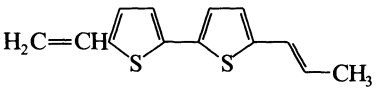
Bp_{20} 88-90°. n_D^{20} 1.5250.

Brown, H.C. *et al*, *J. Org. Chem.*, 1988, **53**, 239 (*synth, ir, pmr, cmr*)

5-(1-Propenyl)-5′-vinyl-2,2′-bithienyl P-80182

5-Ethenyl-5′-(1-propenyl)-2,2′-bithienyl

[17257-06-6]



$C_{13}H_{12}S_2$ M 232.370

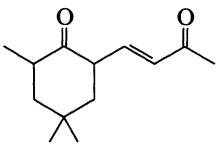
Isol. from above-ground parts of *Bidens connata*. Light-yellow cryst. (pet. ether). Mp 46.5-47°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1228; 1966, **99**, 984 (*isol, uv, ir, pmr, struct, biosynth*)
D'Auria, M. *et al*, *Gazz. Chim. Ital.*, 1986, **116**, 747 (*synth*)

Prosopidione P-80183

2,4,4-Trimethyl-6-(3-oxo-1-butenyl)cyclohexanone, 9CI

[120166-32-7]

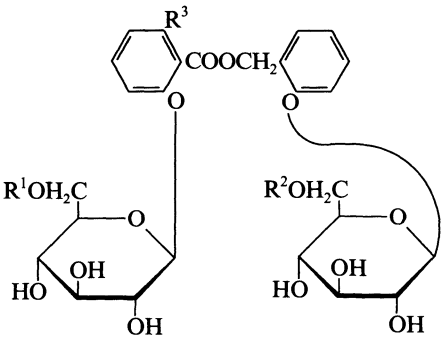


$C_{13}H_{20}O_2$ M 208.300

Constit. of *Prosopis juliflora*. Amorph. powder. Mp 202° dec. $[\alpha]_D$ −19.2° (MeOH).

Ahmad, V.U. *et al*, *Phytochemistry*, 1989, **27**, 278.

Pruyanoside A P-80184



$R^1 = PhCO, R^2 = R^3 = H$

$C_{33}H_{36}O_{15}$ M 672.638

Constit. of *Prunus grayana*. Needles. Mp 195°. $[\alpha]_D^{28}$ −39.6° (c, 0.39 in MeOH).

Shimomura, H. *et al*, *Phytochemistry*, 1989, **28**, 1499.

Pruyanoside B P-80185

As Pruyanoside A, P-80184 with

$R^1 = H, R^2 = PhCO, R^3 = OH$

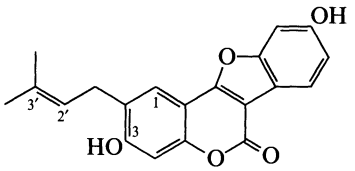
$C_{33}H_{36}O_{16}$ M 688.638

Constit. of *Prunus grayana*. Amorph. powder. $[\alpha]_D^{24}$ −19.3° (c, 1.05 in MeOH).

Shimomura, H. *et al*, *Phytochemistry*, 1989, **28**, 1499.

Psoralidin P-80186

Updated Entry replacing P-02620
3,9-Dihydroxy-2-prenylcoumestan
[18642-23-4]



$C_{20}H_{16}O_5$ M 336.343
Constit. of *Psoralea corylifolia*, *Dolichos biflorus* and *Phaseolus lunatus*. Cryst. (Me_2CO). Mp 290-292° dec.

Di-Ac: Mp 221-223°.

Di-Me ether: Mp 190-191°.

2′,3′-Epoxide: ***Psoralidin oxide***
$C_{20}H_{16}O_6$ M 352.343
Isol. from seeds of *Psoralea corylifolia*. Needles (EtOH). Mp 232-234°. MF incorr. given as $C_{24}H_{20}O_8$.

1-Hydroxy, 3-Me ether: [23013-84-5]. ***Glycyrol***
$C_{21}H_{18}O_6$ M 366.370
Isol. from *Glycyrrhiza* sp. root (licorice). Needles (EtOH). Mp 243.5-245°.

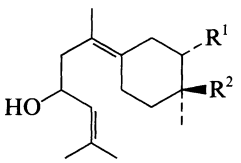
1-Methoxy, 3-Me ether: [23013-85-6]. ***1-O-Methylglycyrol.*** *5-O-Methylglycyrol*
$C_{22}H_{20}O_6$ M 380.396
Isol. from *G.* spp. roots. Needles (Me_2CO). Mp 259-260.5°.

1-Hydroxy, 3-Me ether, di-Ac: Needles (MeOH). Mp 195-196°.

Chakravarti, K.K. *et al*, *CA*, 1948, **42**, 7492 (*isol*)
Khastgir, H.N. *et al*, *Tetrahedron*, 1961, **14**, 275 (*struct*, *uv*, *ir*)
Saitoh, T. *et al*, *Chem. Pharm. Bull.*, 1969, **17**, 729 (*Glycyrol*, 1-*O*-Methylglycyrol)
Gupta, B.K. *et al*, *Phytochemistry*, 1980, **19**, 2232 (*Psoralidin oxide*)
Keen, N.T. *et al*, *Z. Naturforsch.*, *C*, 1980, **35**, 923 (*isol*)

Puertitol A P-80187

[119736-67-3]



R^1 = Br, R^2 = Cl

$C_{15}H_{24}BrClO$ M 335.711
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ −37° (c, 1.62 in $CHCl_3$).

Vazquez, J.T. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1257 (*isol*, *pmr*, *cmr*, *cd*)

Puertitol B P-80188

[119736-69-5]

As Puertitol A, P-80187 with

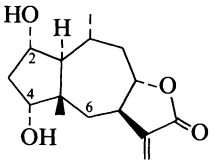
R^1 = Cl, R^2 = Br

$C_{15}H_{24}BrClO$ M 335.711
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +66° (c, 0.25 in $CHCl_3$).

Vazquez, J.T. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1257 (*isol*, *pmr*, *cmr*, *cd*)

Pulchellin A P-80189

Updated Entry replacing P-70138
Pulchellin
[6754-35-4]



$C_{15}H_{22}O_4$ M 266.336
Constit. of *Gaillardia pulchella*. Cryst. (EtOAc). Mp 166-167°. $[\alpha]_D^{26}$ −36.2° (c, 2.43 in $CHCl_3$).

2,4-Di-Ac: [23754-36-1]. ***Pulchellin diacetate***
$C_{19}H_{26}O_6$ M 350.411
From *Loxochysanus sinuatus*. Oil.

2-O-(3-Methylbutanoyl): ***Pulchellin 2-O-isovalerate***
$C_{20}H_{32}O_5$ M 352.470
From *L. sinuatus*. Oil. $[\alpha]_D^{26}$ −13° (c, 0.43 in $CHCl_3$).

2-Tigloyl: [97605-30-6]. ***Pulchellin 2-O-tiglate***
$C_{20}H_{28}O_5$ M 348.438
From *L. sinuatus*. Oil.

6β-Hydroxy, 2-(3-Methylbutanoyl): [97605-31-7]. ***6β-Hydroxypulchellin 2-O-isovalerate***
$C_{20}H_{30}O_6$ M 366.453
From *L. sinuatus*. Cryst. Mp 127°.

6β-Hydroxy, 2-Ac: [97643-92-0]. ***6β-Hydroxypulchellin 2-O-acetate***
$C_{17}H_{24}O_6$ M 324.373
From *L. sinuatus*. Cryst. Mp 87°. $[\alpha]_D^{24}$ +14° (c, 0.97 in MeOH).

4-Epimer: ***4-Epipulchellin***
$C_{15}H_{24}O_4$ M 268.352
Constit. of *G. pulchella*. Oil.

4-Epimer, di-Ac: Cryst. Mp 133-134°.

6α-Hydroxy: ***6α-Hydroxypulchellin***
$C_{15}H_{22}O_5$ M 282.336
Constit. of *G. pulchella*.

6α-Hydroxy, O^4-angeloyl: ***6α-Hydroxypulchellin 4-O-angelate***
$C_{20}H_{28}O_6$ M 364.438
Constit. of *G. pulchella*.

6β-Acetoxy, O^4-angeloyl: ***6β-Acetoxypulchellin 4-O-angelate***
$C_{22}H_{30}O_7$ M 406.475
Constit. of *G. pulchella*.

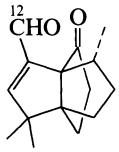
2-Deoxy, 4-epimer: ***2-Deoxy-4-epipulchellin***
$C_{15}H_{22}O_3$ M 250.337
Constit. of *Ondetia linearis*. Cryst. Mp 135°. $[\alpha]_D^{24}$ +43° (c, 0.59 in $CHCl_3$).

Herz, W. *et al*, *Tetrahedron*, 1963, **19**, 483 (*isol*, *uv*, *ir*, *pmr*)
Aota, K. *et al*, *J. Org. Chem.*, 1970, **35**, 1448 (*isol*)
Inayama, S. *et al*, *Heterocycles*, 1985, **23**, 377 (*synth*)
Bohlmann, F. *et al*, *Phytochemistry*, 1985, **24**, 1021 (*isol*)
Harimaya, K. *et al*, *Heterocycles*, 1988, **27**, 83 (*epimer*)
Yu, S. *et al*, *Phytochemistry*, 1988, **27**, 2887 (*derivs*)
Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 1653 (*derivs*)

Pulicaral P-80190

*5,6-Dihydro-1,1,4-trimethyl-9-oxo-1*H,*4*H-*3*a,*6*a-*propanopentalene-3-carboxaldehyde, 9CI*

[119767-05-4]



$C_{15}H_{20}O_2$ M 232.322

Constit. of *Pulicaria paludosa*. Cryst. (CH_2Cl_2). Mp 70°. $[\alpha]_D^{24}$ −58.9° (c, 0.3 in $CHCl_3$).

12-Carboxylic acid: [119767-06-5]. ***Pulicaric acid***

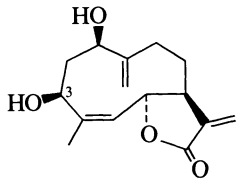
$C_{15}H_{20}O_3$ M 248.321

Constit. of *P. paludosa*. Oil. $[\alpha]_D^{24}$ −57.6° (c, 0.7 in $CHCl_3$).

San Feliciano, A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1153 (*isol, pmr, cmr*)

Pulverulide P-80191

Updated Entry replacing P-30207



$C_{15}H_{20}O_4$ M 264.321

Constit. of *Leucanthemopsis pulverulenta*. Oil. $[\alpha]_D$ +8.4° (c, 0.83 in $CHCl_3$).

3-Ac: ***3-Acetylpulverulide***

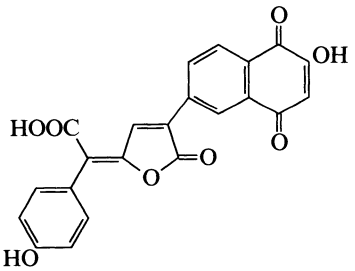
$C_{17}H_{22}O_5$ M 306.358

Constit. of *Stevia alpina*. Gum.

De Pascual Teresa, J. *et al*, *Phytochemistry*, 1984, **23**, 1178 (*isol, struct*)

de Heluani, C.S. *et al*, *Phytochemistry*, 1989, **28**, 1931 (*deriv*)

Pulviquinone A P-80192



$C_{22}H_{12}O_9$ M 420.331

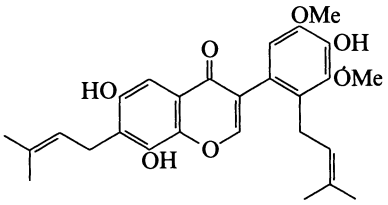
Pigment from the bay boletus *Xerocomus badius*. λ_{max} 265sh, 278, 312, 354, 422 nm. Isol. as the Me ester, an artifact of methylation.

[90295-71-9]

Steffan, B. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 445 (*isol, struct*)

Pumilaisoflavone C P-80193

4′,6,8-Trihydroxy-3′,5′-dimethoxy-2′,7-diprenylisoflavone

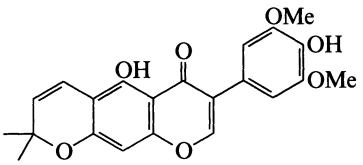


$C_{27}H_{30}O_7$ M 466.530

Constit. of *Tephrosia pumila*. Needles (MeOH). Mp 180-182°.

Yenesew, A. *et al*, *Phytochemistry*, 1989, **28**, 1291.

Pumilaisoflavone D P-80194



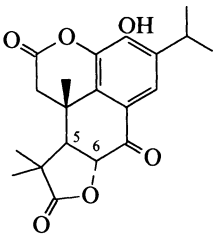
$C_{22}H_{20}O_7$ M 396.396

Constit. of *Tephrosia pumila*. Needles (MeOH). Mp 174-176°.

Yenesew, A. *et al*, *Phytochemistry*, 1989, **28**, 1291.

Pygmaeocin A P-80195

[122590-05-0]



$C_{20}H_{22}O_6$ M 358.390

Constit. of *Pygmaeopremna herbacea*. Cryst. (MeOH). Mp 281-283°.

5,6-Didehydro: [122590-06-1]. *5,6-Didehydropygmaeocin A*

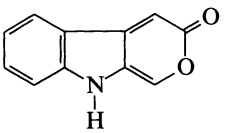
$C_{20}H_{20}O_6$ M 356.374

Constit. of *P. herbacea*. Yellow cryst. (MeOH). Mp 211-213°.

Chen, W. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 581 (*isol, pmr, cmr*)

Pyrano[3,4-*b*]indol-3(9*H*)-one, 9CI P-80196

[4375-21-7]



$C_{11}H_7NO_2$ M 185.182

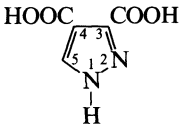
Mp *ca.* 165° (darkens). Numerous 1-subst. derivs. prepared.

Moody, C.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1407 (*synth, ir, pmr, ms*)

1*H*-Pyrazole-3,4-dicarboxylic acid, 9CI P-80197

Updated Entry replacing P-02758

[35344-99-1]



$C_5H_4N_2O_4$ M 156.098

Needles + $1H_2O$ (dil. HNO_3). Mp >300° (anhyd.), Mp 260° dec. (monohydrate). Forms gels on pptn. from H_2O.

Di-Me ester: [33090-46-9].
$C_7H_8N_2O_4$ M 184.151
Needles (C_6H_6/pet. ether). Mp 141°.

Diamide: [21272-56-0].
$C_5H_6N_4O_2$ M 154.128
Cryst. (AcOH). Mp 260° dec.

Dinitrile: [33146-98-4]. *3,4-Dicyanopyrazole*
$C_5H_2N_4$ M 118.098
Cryst. (EtOAc/pet. ether). Mp 194°.

N-*Ac:*
$C_7H_6N_2O_5$ M 198.135
Mp 169°.

3-Et ester:
$C_7H_8N_2O_4$ M 184.151
Cryst. (EtOH). Mp 263° dec.

1-Benzyl, di-Me ester: [7189-02-8].
$C_{14}H_{14}N_2O_4$ M 274.276
Light yellow oil. $Bp_{.001}$ 185°.

1-Me, di-Et ester: [10514-60-0].
$C_{10}H_{14}N_2O_4$ M 226.232
Yellow oil. $Bp_{0.5}$ 135-145°.

1-Me: [10505-21-2].
$C_6H_6N_2O_4$ M 170.124
Cryst. (H_2O). Mp 239-241° (233°).

1-Me, di-Me ester: [22050-80-2].
$C_8H_{10}N_2O_4$ M 198.178
Needles (pet. ether). Mp 68-69° (67°).

4-Me ester, 3-nitrile: [33090-69-6]. *Methyl 3-cyanopyrazole-4-carboxylate*
$C_6H_5N_3O_2$ M 151.124
Cryst. (EtOAc/pet. ether). Mp 186°.

1-Benzyl: [19311-81-0].
$C_{12}H_{10}N_2O_4$ M 246.222
Mp 195.5-197° dec.

Di-Et ester: [37687-26-6].
$C_9H_{12}N_2O_4$ M 212.205
Cryst. (C_6H_6/pet. ether). Mp 69-70°.

[34982-39-3]

Jones, R.G. *et al*, *J. Org. Chem.*, 1955, **20**, 1342 (*synth, Et esters*)
Acheson, R.M. *et al*, *J. Chem. Soc.*, 1963, 1008 (*Me ester*)
Huisgen, R. *et al*, *Chem. Ber.*, 1968, **101**, 536 (*N-Ph, N-Benzyl*)
Bastide, J. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 1336 (*nitriles, amide, N-Me*)
Greco, C.V. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 720 (*esters*)
Winter, W. *et al*, *Chem. Ber.*, 1974, **107**, 2127 (*N-Me*)

1*H*-Pyrazole-3,5-dicarboxylic acid, 9CI P-80198

Updated Entry replacing P-02759

Mp >360°.

Monohydrate: Needles (HCl aq.). Mp 287-290° dec.

Di-Me ester: [4077-76-3].
$C_7H_9N_2O_4$ M 185.159
Plates (Et_2O). Mp 151-155°.

N-*Me:* [75092-39-6].
$C_6H_6N_2O_4$ M 170.124
Prisms (H_2O). Mp 266-268° (249.5-250° dec.).

N-*Me, 3-Me ester:* [117860-55-6].
$C_7H_8N_2O_4$ M 184.151
Needles (MeOH aq.). Mp 129-130.5°.

N-*Me, 5-Me ester:* [117860-56-7].
$C_7H_8N_2O_4$ M 184.151
Cryst. (EtOAc). Mp 172-172.5°.

N-*Me, Di-Me ester:* [33146-99-5].
$C_8H_{10}N_2O_4$ M 198.178
Needles (pet. ether). Mp 72-73.5°.

N-*Et:*
$C_7H_8N_2O_4$ M 184.151
Mp 243°.

N-*Et, Di-Me ester:*
$C_8H_{10}N_2O_4$ M 198.178
Mp 66°.

N-*Ac, Di-Me ester:*
$C_9H_{10}N_2O_5$ M 226.188
Mp 84.5-85°.

Di-Et ester: [37687-24-4].
$C_9H_{12}N_2O_4$ M 212.205
Cryst. (C_6H_6/EtOAc). Mp 49-51°.

Buchner, E. *et al*, *Justus Liebigs Ann. Chem.*, 1893, **273**, 232, 246 (*synth, Di-Me ester*)
Knorr, L. *et al*, *Justus Liebigs Ann. Chem.*, 1894, **279**, 218.
Gray, T., *Ber.*, 1900, **33**, 1220.
v. Auwers, K. *et al*, *J. Prakt. Chem.*, 1930, **126**, 196; 177 (*N-Ac*)
Eidebenz, E. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1943, **281**, 171 (*N-Et derivs, amides*)
Daeniker, H.U. *et al*, *Helv. Chim. Acta*, 1963, **46**, 805 (*amide-ester*)
Makabe, O. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 3210 (*Di-Et ester*)
Denny, W.A., *J. Org. Chem.*, 1989, **54**, 428 (*synth, N-Me and esters*)

1*H*-Pyrazole-4,5-dicarboxylic acid P-80199

[31962-35-3]

$C_5H_4N_2O_4$ M 156.098

1-Unsubstituted derivs. tautomeric with the 3,4-dicarboxylic acid,

1-Me: [10505-19-8].
$C_6H_6N_2O_4$ M 170.124
Cryst. (H_2O). Mp 182-184° (176-177°). Early work refers to a dihydrate, mp. 233-235°; this is apparently incorrect.

1-Me, Di-Me ester: [33090-52-7].
$C_8H_{10}N_2O_4$ M 198.178
Cryst. (pet. ether). Mp 32-33°.

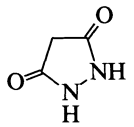
1-Me, Di-Et ester: [10514-61-1].
$C_{10}H_{14}N_2O_4$ M 226.232
Oil. $Bp_{0.5}$ 100-105°.

Bauer, L. *et al*, *J. Org. Chem.*, 1966, **31**, 2491 (*N*-Me, Et ester)
Winter, W. *et al*, *Chem. Ber.*, 1974, **107**, 2127 (*N*-Me)

3,5-Pyrazolidinedione, 9CI, 8CI P-80200

N,N′-*Malonylhydrazine*

[4744-71-2]



$C_3H_4N_2O_2$ M 100.077
Cryst. (MeOH). Mp 290° dec.

1-Ph: [19933-22-3].
$C_9H_8N_2O_2$ M 176.174
Yellow plates (EtOH). Mp 192°.

1,2-Dipropyl: [93847-23-5].
$C_9H_{16}N_2O_2$ M 184.238
Yellow, oily solid.

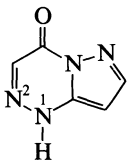
1,2-Dibenzyl: [93847-22-4].
$C_{17}H_{16}N_2O_2$ M 280.326
Yellow cryst. (MeCN). Mp 128.5°.

1,2-Di-Ph: [2652-77-9].
$C_{15}H_{12}N_2O_2$ M 252.272
Plates (EtOH). Mp 178-179°.

Conrad, M. *et al*, *Chem. Ber.*, 1906, **39**, 2283 (*phenyl*)
McGee, M.A. *et al*, *J. Chem. Soc.*, 1960, 1989 (*diphenyl*)
Selva, A. *et al*, *Org. Mass Spectrom.*, 1975, **10**, 606 (*ms, deriv*)
Dubau, F.-P., *Chem. Ber.*, 1983, **116**, 2714 (*synth, pmr*)
Fritsch, G. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1986, **319**, 70 (*synth, cryst struct*)
Lawton, G. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 877 (*derivs, synth, ir, pmr*)

Pyrazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one P-80201

[112298-50-7]



$C_5H_4N_4O$ M 136.113
Mp >300°.

1-Me: [112298-53-0].
$C_6H_6N_4O$ M 150.140
Mp 185-187°.

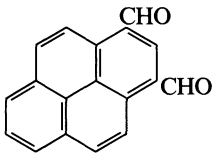
2-Me: [112298-54-1].
$C_6H_6N_4O$ M 150.140
Mp 180-183°. Zwitterionic.

Farràs, J. *et al*, *J. Org. Chem.*, 1988, **53**, 887 (*synth, pmr, cmr*)

1,3-Pyrenedicarboxaldehyde P-80202

1,3-Diformylpyrene

[120915-14-2]



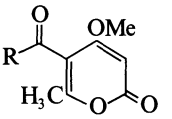
$C_{18}H_{10}O_2$ M 258.276
Yellow needles (CH_2Cl_2). Mp 245-246° (sealed tube).

Goltz, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3767 (*synth, uv, ms, pmr*)

Pyrenocine A P-80203

*4-Methoxy-6-methyl-5-(1-oxo-2-butenyl)2-*H*-pyran-2-one, 9CI. Citreopyrone*

[76868-97-8]



(*E*)-*form*

R = $H_3CCH{=}CH$

$C_{11}H_{12}O_4$ M 208.213
Formerly assigned furanoid struct. Isol. from *Pyrenochaeta terrestris* and *Penicillium citreoviride* and *Alternaria* sp. nov. Plant growth inhibitor. Cryst. (MeOH). Mp 110.9-111.6°.

1′-Alcohol: [94474-69-8]. ***Pyrenocine C***
$C_{11}H_{14}O_4$ M 210.229
From *P. terrestris*. Weak phytotoxin. Needles (Et_2O). Mp 81.5-82.0°. $[\alpha]_D^{20}$ +0.3° (c, 0.37 in $CHCl_3$). Virtually racemic.

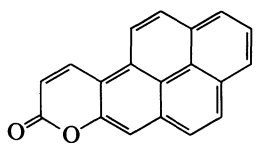
2′,3′-Dihydro, 3′-hydroxy: [72674-29-4]. ***Pyrenocine B***
$C_{11}H_{14}O_5$ M 226.229
Metab. of *P. terrestris*. Phytotoxin. Cryst. (Et_2O/hexane). Mp 103-103.5°.

[72674-30-7]

Sato, H. *et al*, *Agric. Biol. Chem.*, 1979, **43**, 2409 (*isol*)
Niwa, M. *et al*, *Tetrahedron Lett.*, 1980, 4483 (*isol*)
Sato, H. *et al*, *Agric. Biol. Chem.*, 1981, **45**, 795 (*cryst struct*)
Sparace, S.A. *et al*, *Phytochemistry*, 1984, **23**, 2693 (*deriv*)
Shizuri, Y. *et al*, *Tetrahedron Lett.*, 1984, **25**, 1583 (*biosynth*)
Tal, B. *et al*, *Z. Naturforsch.*, *C*, 1986, **41**, 1032 (*isol*)
Sporace, S.A. *et al*, *Can. J. Microbiol.*, 1987, **33**, 327 (*props*)
Ichihara, A. *et al*, *Tetrahedron*, 1987, **43**, 5245 (*synth*)

8*H*-Pyreno[2,1-*b*]pyran-8-one P-80204

[115560-48-0]

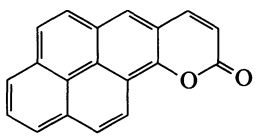


$C_{19}H_{10}O_2$ M 270.287
Cryst. Mp 245-246°.

Harvey, R.G. *et al*, *J. Org. Chem.*, 1988, **53**, 3936 (*synth, pmr*)

9*H*-Pyreno[1,2-*b*]pyran-9-one P-80205

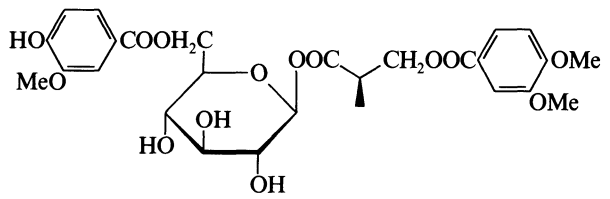
[115560-47-9]



$C_{19}H_{10}O_2$ M 270.287
Cryst. (C_6H_6/hexane). Mp 208-209°.

Harvey, R.G. *et al*, *J. Org. Chem.*, 1988, **53**, 3936 (*synth, pmr*)

Pyrenoside P-80206

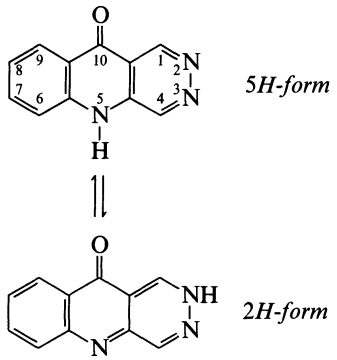


$C_{27}H_{32}O_{14}$ M 580.541
Constit. of *Gentiana pyrenaica*. Amorph. powder.

Garcia, J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 996 (*isol, pmr, cmr*)

Pyridazino[4,5-*b*]quinolin-10(5*H*)-one, 9CI P-80207

[115276-33-0]



5H-form

2H-form

$C_{11}H_7N_3O$ M 197.196

5H-form

Solid (DMF/MeOH). Mp >300° dec.

5-Me: [115276-39-6].
$C_{12}H_9N_3O$ M 211.223
Pale yellow cryst. (butanone). Mp 279-280°.

5-Et: [115276-40-9].
$C_{13}H_{11}N_3O$ M 225.249
Pale yellow needles (Me_2CO/diisopropyl ether). Mp 214-215°.

2H-form

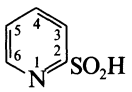
2-Me: [115276-34-1].
$C_{12}H_9N_3O$ M 211.223
Yellow needles (propanol). Mp 275-278° dec.

2-Benzyl: [115276-35-2].
$C_{18}H_{13}N_3O$ M 287.320
Yellow needles (EtOH). Mp 240-243°.

Haider, N. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 401 (*synth, deriv, pmr, ir, uv*)

2-Pyridinesulfinic acid P-80208

[24367-66-6]



$C_5H_5NO_2S$ M 143.166
Obt. as cryst. Na salt.

Kamiyama, T. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 2652.

4-Pyridinesulfinic acid P-80209

[116008-37-8]

$C_5H_5NO_2S$ M 143.166
Obt. as cryst. Na salt.

Kamiyama, T. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 2652.

Pyridinium fluorochromate P-80210

$C_5H_5NH^{\oplus}\ CrO_3F^{\ominus}$

$C_5H_6CrFNO_3$ M 199.102
Selective oxidising agent. Bright orange cryst. (106-108°).

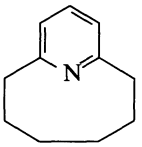
▷ Hazardous synth.

Bhattacharjee, M.N. *et al*, *Synthesis*, 1982, 588 (*synth.*)
Bhattacharjee, M.N. *et al*, *Tetrahedron*, 1987, **43**, 5389 (*use*)

[6](2,6)Pyridinophane P-80211

12-Azabicyclo[6.3.1]dodeca-1(12),8,10-triene, 9CI.
[6](2,6)Pyridophane

[56912-79-9]



$C_{11}H_{15}N$ M 161.246
Oil. $Bp_{1.9}$ 65°.

B,HClO$_4$: Mp 90-93° (77-78°).

N-*Oxide:* [118537-97-6].
$C_{11}H_{15}NO$ M 177.246
Cryst. (pentane). Mp 83°.

Weber, H. *et al*, *Chem. Ber.*, 1985, **118**, 4259; 1989, **122**, 945.

[7](2,6)Pyridinophane P-80212

13-Azabicyclo[7.3.1]trideca-1(13),9,11-triene, 9CI.
[7](2,6)Pyridophane

[22776-72-3]

$C_{12}H_{17}N$ M 175.273
Oil. $Bp_{1.5}$ 90-100°.

B,HClO$_4$: Mp 132-133°.

N-Oxide: [118537-98-7].
$C_{12}H_{17}NO$ M 191.272
Cryst. (pentane). Mp 63-65°.

Weber, H. *et al*, *Chem. Ber.*, 1985, **118**, 4259; 1989, **122**, 945.

[8](2,6)Pyridinophane P-80213

14-Azabicyclo[8.3.1]tetradeca-1(14),10,12-triene, 9CI.
[8](2,6)Pyridophane

[56912-80-2]

$C_{13}H_{19}N$ M 189.300
Oil. $Bp_{1.0}$ 100-110°.

B,HClO$_4$: Mp 181-182°.

N-*Oxide:* [118537-99-8].
$C_{13}H_{19}NO$ M 205.299
Cryst. (pentane). Mp 76°.

Weber, H. *et al*, *Chem. Ber.*, 1985, **118**, 4259; 1989, **122**, 945.

[9](2,6)Pyridinophane P-80214

15-Azabicyclo[9.3.1]pentadeca-1(15),11,13-triene, 9CI.
[9](2,6)Pyridophane

[56929-81-8]

$C_{14}H_{21}N$ M 203.327

$Bp_{1.0}$ 120-130°.

B,HClO$_4$: Mp 174°.

N-*Oxide:*

$C_{14}H_{21}NO$ M 219.326

Cryst. (pentane). Mp 70°.

Weber, H. *et al*, *Chem. Ber.*, 1985, **118**, 4259; 1989, **122**, 945.

[10](2,6)Pyridinophane P-80215

16-Azabicyclo[10.3.1]hexadeca-1(16),12,14-triene, 9CI.

[10](2,6)Pyridophane

[4432-68-2]

$C_{15}H_{23}N$ M 217.353

Oil. $Bp_{1.5}$ 140°.

B,HClO$_4$: Mp 174-175°.

N-*Oxide:* [118538-01-5].

$C_{15}H_{23}NO$ M 233.353

Cryst. (pentane). Mp 78-80° (73-74°).

Weber, H. *et al*, *Chem. Ber.*, 1985, **118**, 4259; 1989, **122**, 945.

[12](2,6)Pyridinophane P-80216

18-Azabicyclo[12.3.1]octadeca-1(18),14,16-triene, 9CI.

[12](2,6)Pyridophane

[56912-81-3]

$C_{17}H_{27}N$ M 245.407

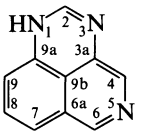
$Bp_{1.2}$ 170-190°.

B,HClO$_4$: Cryst. (Me_2CO/Et_2O). Mp 146-148°.

Weber, H. *et al*, *Chem. Ber.*, 1985, **118**, 4259.

1*H*-Pyrido[3,4,5-*de*]quinazoline P-80217

[110748-36-2]



$C_{10}H_7N_3$ M 169.185

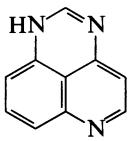
Yellow cryst. (MeOH aq.). Mp 246-249°.

Woodgate, P.D. *et al*, *Heterocycles*, 1987, **26**, 1029 (*synth, pmr, ms*)

1*H*-Pyrido[4,3,2-*de*]quinazoline P-80218

6-Azaperimidine

[111493-32-4]



$C_{10}H_7N_3$ M 169.185

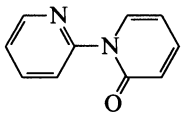
Bright yellow needles by subl. Mp 241-244° dec.

Woodgate, P.D. *et al*, *Heterocycles*, 1987, **26**, 1029 (*synth, ir, pmr, ms*)

1-(2-Pyridyl)-2-pyridone P-80219

[1(2H),2'-Bipyridin]-2-one, 8CI

[3480-65-7]



$C_{10}H_8N_2O$ M 172.186

Needles (pet. ether). Mp 55°. $Bp_{0.7}$ 120-130°.

Picrate: Mp 116-118°.

Ramirez, F. *et al*, *Chem. Ind.* (*London*), 1957, 46 (*synth*)
de Villiers, P.A. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1957, **76**, 647 (*synth, uv*)
Wibaut, J.P. *et al*, *Bull. Soc. Chim. Fr.*, 1958, 424 (*synth*)
Ramirez, F. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 156 (*synth, ir, uv*)
von Ostwalden, P.W. *et al*, *J. Org. Chem.*, 1971, **36**, 3792 (*synth, pmr*)
Del Giudice, M.R. *et al*, *Tetrahedron*, 1984, **40**, 4067 (*ir, pmr*)

1-(2-Pyridyl)-4-pyridone P-80220

[1(4H),2'-Bipyridin]-4-one, 9CI

[76520-27-9]

$C_{10}H_8N_2O$ M 172.186

Needles (C_6H_6). Mp 164-165°.

de Villiers, P.A. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1957, **76**, 647 (*synth, uv*)
Matsumura, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 2891; 1984, **57**, 1961 (*synth*)

1-(3-Pyridyl)-4-pyridone P-80221

[1(4H),3'-Bipyridin]-4-one, 9CI

[34847-11-5]

$C_{10}H_8N_2O$ M 172.186

Cryst. ($CHCl_3$). Mp 189-191°.

B, 2HCl: [34847-10-4].

Needles (H_2O). Mp 192-195°.

Fleet, G.W.J. *et al*, *J. Chem. Soc. C*, 1971, 3948 (*synth, ms, pmr*)

1-(4-Pyridyl)-2-pyridone P-80222

[1(2H),4'-Bipyridin]-2-one

[62150-42-9]

$C_{10}H_8N_2O$ M 172.186

Blunt needles (C_6H_6). Mp 155-158°. $Bp_{0.1}$ 125-135°.

de Villiers, P.A. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1957, **76**, 647 (*synth, deriv*)
Witek, W., *Pol. J. Chem.* (*Rocz. Chem.*), 1976, **50**, 1625 (*synth*)

1-(4-Pyridyl)-4-pyridone P-80223

[1(4H),4'-Bipyridin]-4-one

[3881-38-7]

$C_{10}H_8N_2O$ M 172.186

Cryst. (C_6H_6, EtOH, or Me_2CO/pet. ether). Mp 177-178°. Forms a monohydrate.

B, 2HCl: Mp 185-187°.

Thyagarajan, B. *et al*, *Chem. Ber.*, 1966, **99**, 368 (*synth, ir, uv*)
Oae, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 1420 (*synth*)
Kobayashi, Y. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 2489 (*synth, pmr, uv*)
Fleet, G.W.J. *et al*, *J. Chem. Soc. C*, 1971, 3948 (*synth, pmr*)
Kappe, T. *et al*, *Monatsh. Chem.*, 1972, **103**, 426 (*synth, ir*)
Del Giudice, M.R. *et al*, *Tetrahedron*, 1984, **40**, 4067 (*cmr, ir, pmr*)

3,4-Pyridyne P-80224

3,4-Didehydropyridine, 9CI

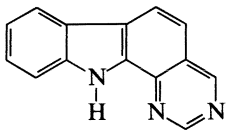
[7129-66-0]

C_5H_3N M 77.085

Transient intermediate. Obs. by ir at 13K in N_2 or Ar matrices.

Reinecke, M.G., *Tetrahedron*, 1982, **38**, 427 (*rev*)
Nam, H.-H. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4096 (*synth, ir*)

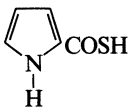
11*H*-Pyrimidino[4,5-*a*]carbazole P-80225



$C_{14}H_9N_3$ M 219.245
Yellow cryst. Mp 218°.

Ganzengel, J.M. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 1500 (*synth*)

2-Pyrrolethiolcarboxylic acid P-80226

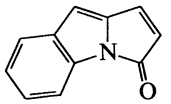


C_5H_5NOS M 127.167
Me ester: [118792-46-4].
C_6H_7NOS M 141.193
Cryst. (pet. ether). Mp 79-80°.
1-Me, Me ester: [118792-47-5].
C_7H_9NOS M 155.220
Liq. Bp_{24} 131-132°.

Barbero, M. *et al*, *Synthesis*, 1988, 300 (*synth, pmr, cmr, ir*)

3*H*-Pyrrolo[1,2-*a*]indol-3-one P-80227

[24009-76-5]

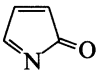


$C_{11}H_7NO$ M 169.182
Cryst. by subl. Mp 94-95°.

Auerbach, J. *et al*, *J. Org. Chem.*, 1971, **36**, 31 (*synth*)
Flitsch, W. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 239 (*synth*)

2*H*-Pyrrol-2-one P-80228

2-Aza-2,4-cyclopentadienone



C_4H_3NO M 81.074
Transient species, which acts as diene or dienophile in Diels-Alder reactions.

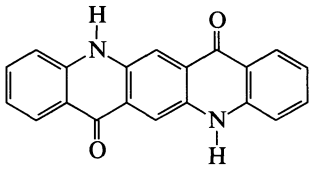
Gaviña, F. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4017.

Q

Quinacridone — Q-80001

*5,12-Dihydroquino[2,3-*b*]acridine-7,14-dione.* lin-trans-*Quinacridone. CI Pigment Violet 19*

[1047-16-1]



$C_{20}H_{12}N_2O_2$ M 312.327

Pigment, and parent of a family of pigments. Red-violet cryst., yellow in vapour phase. Insol. most solvents. Mp 390°.

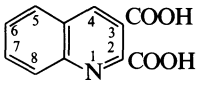
Labana, S.S. *et al*, *Chem. Rev.*, 1967, **67**, 1 (*rev, uv*)
Kimura, S., *Makromol. Chem.*, 1968, **117**, 203 (*synth, ir*)
Chung, F.H. *et al*, *J. Appl. Crystallogr.*, 1971, **4**, 506 (*cryst struct*)
Altiparmakian, R.H. *et al*, *Helv. Chim. Acta*, 1972, **55**, 85 (*pmr*)
Yokoyama, Y., *Bull. Chem. Soc. Jpn.*, 1983, **56**, 1775 (*pmr, uv*)

2,3-Quinolinedicarboxylic acid, 9CI — Q-80002

Updated Entry replacing Q-40004

Acridinic acid

[643-38-9]



$C_{11}H_7NO_4$ M 217.181

Needles + 2 or $3H_2O$ (H_2O or EtOH). Spar. sol. cold H_2O, Et_2O, sol. EtOH. Loses CO_2 at 105°.

Di-Me ester: [17507-03-8].
$C_{13}H_{11}NO_4$ M 245.234
Prisms (MeOH or C_6H_6). Mp 107-108°.

Di-Et ester: [32413-08-4].
$C_{15}H_{15}NO_4$ M 273.288
Cryst. (hexane). Mp 54-55°.

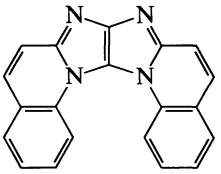
Di-Et ester, N-*oxide:* [92525-68-3].
$C_{15}H_{15}NO_5$ M 289.287
Cryst. ($CHCl_3$/diisopropyl ether). Mp 111-112°.

Anhydride: [4945-42-0].
$C_{11}H_5NO_3$ M 199.165
Mp 225°.

Imide:
$C_{11}H_6N_2O_2$ M 198.181
Mp 316°.

Moriconi, E.J. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 38 (*synth*)
Godard, A. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 906 (*synth*)
Kadin, S.B. *et al*, *J. Org. Chem.*, 1984, **49**, 4999 (*derivs*)
Ladner, D.W., *Synth. Commun.*, 1986, **16**, 157 (*synth*)
Maulding, D.R., *J. Heterocycl. Chem.*, 1988, **25**, 1777 (*synth, bibl*)

Quinolino[1″,2″:1′,2′]imidazo[4′,5′:4,5]imidazo[1,2-*a*]quinoline — Q-80003



$C_{20}H_{12}N_4$ M 308.342

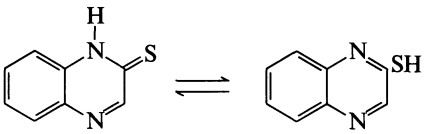
Solid + $\frac{1}{2}H_2O$. Mp >250°.

Pereira, D.E. *et al*, *Tetrahedron*, 1987, **43**, 4931 (*synth, pmr, cmr, uv, ms*)

2-(1*H*)-Quinoxalinethione — Q-80004

2-Mercaptoquinoxaline. 2-Quinoxalinethiol

[6962-54-5]

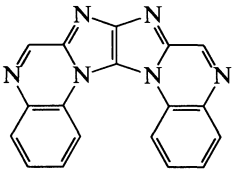


$C_8H_6N_2S$ M 162.215

Orange needles (MeOH). Mp 204-205°.

Wolf, F.J. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2266 (*synth*)
Ijima, C. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 618 (*synth, pmr*)

Quinoxalino[1″,2″:1′,2′]imidazo[4′,5′:4,5]imidazo[1,2-*a*]quinoxaline — Q-80005



$C_{18}H_{10}N_6$ M 310.317

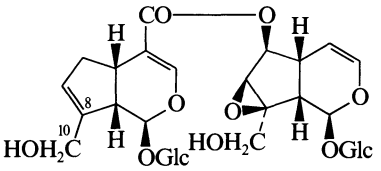
Solid. Mp >250°.

Pereira, D.E. *et al*, *Tetrahedron*, 1987, **43**, 4931 (*synth, pmr, cmr, ir, uv, ms*)

R

Radiatoside B — R-80001

[111514-49-9]



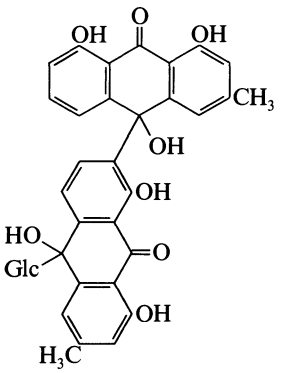
$C_{31}H_{42}O_{19}$ M 718.661
Constit. of *Argylia radiata*. Amorph. powder. $[\alpha]_D^{20}$ −138.6° (c, 1 in MeOH).

10-Deoxy, $\Delta^{8,10}$-isomer: [111514-50-2]. ***Radiatoside C***
$C_{31}H_{42}O_{18}$ M 702.662
Constit. of *A. radiata*. Amorph. powder. $[\alpha]_D^{20}$ −125.3° (c, 1 in MeOH).

Bianco, A. *et al*, *Planta Med.*, 1987, **53**, 385.

Ramosin — R-80002

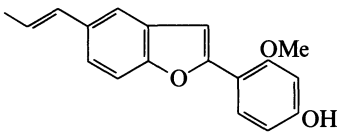
[120163-26-0]



$C_{36}H_{32}O_{13}$ M 672.641
Constit. of *Asphodelus ramosus*. Yellow amorph. solid. $[\alpha]_D$ −74° (c, 1.1 in MeOH).

Adinolfi, M. *et al*, *Phytochemistry*, 1989, **28**, 284.

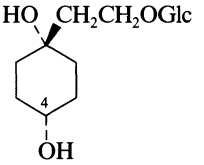
Ratanhiaphenol III — R-80003



$C_{19}H_{18}O_3$ M 294.349
Constit. of *Krameria lanceolata*. Cryst. Mp 134-135°.

Achenbach, H. *et al*, *Phytochemistry*, 1989, **28**, 1959.

Rengyoside A — R-80004



$C_{14}H_{26}O_8$ M 322.355
Constit. of *Forsythia suspensa*. Amorph. solid. $[\alpha]_D^{23}$ −11° (c, 0.18 in MeOH).

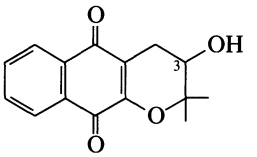
4-Ketone: ***Rengyoside* B**
$C_{14}H_{24}O_8$ M 320.339
Constit. of *F. suspensa*. Amorph. solid. $[\alpha]_D^{23}$ −10.4° (c, 0.28 in EtOH).

6′-(4-Hydroxyphenylacetyl): ***Rengyoside* C**
$C_{22}H_{32}O_{10}$ M 456.489
Constit. of *F. suspensa*. Powder. $[\alpha]_D^{23}$ −21.9° (c, 0.06 in 2-propanol).

Seya, K. *et al*, *Phytochemistry*, 1989, **28**, 1495.

Rhinacanthin A — R-80005

[119626-45-8]



$C_{15}H_{14}O_4$ M 258.273
Constit. of *Rhinacanthus nasutus* roots. Orange needles (Me_2CO). Mp 186.5-187°. $[\alpha]_D$ −12.9° (c, 0.25 in $CHCl_3$).

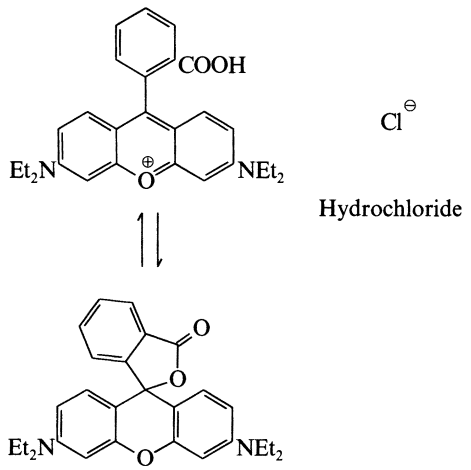
O-*(2,6-Dimethyl-2,6-octadienoyl):* [119626-46-9]. ***Rhinacanthin B***
$C_{25}H_{28}O_5$ M 408.493
Constit. of *R. nasutus* roots. Shows cytotoxic activity. Pale yellow needles (hexane). Mp 78-80°. $[\alpha]_D$ −47.9° (c, 0.24 in $CHCl_3$).

Wu, T.-S. *et al*, *Phytochemistry*, 1988, **27**, 3787.

Rhodamine B R-80006

N-[[9-(2-Carboxyphenyl)-6-diethylamino]-3H-xanthen-3-ylidene]-N-ethyl ethanaminium, 9CI. [9-(o-Carboxyphenyl)-6-(diethylamino)-3H-xanthen-3-ylidene]diethylammonium, 8CI. 9-(2-Carboxyphenyl)-3,6-bis(diethylamino)xanthylium. CI Basic Violet 10. CI Solvent red 49

[14899-08-2]



$C_{28}H_{31}N_2O_3^{\oplus}$ M 443.564

Dyestuffs for cosmetics, drugs, fluorescent inks, chemical lasers. Used in detn. of metals. Colourless prisms (EtOH)(anhyd.). Green leaflets + $4H_2O$ (H_2O). Mp 165°. Red soln. with green fluor. in H_2O or EtOH, colourless in Et_2O, C_6H_6.

Hydrochloride: [81-88-9].
Important dyestuff. Shining metallic-lustred leaflets (dil. HCl). V. sol. H_2O, EtOH; sol. C_6H_6; sl. sol. dil. HCl. Forms red solution in H_2O, strongly fluorescent orange-yellow.

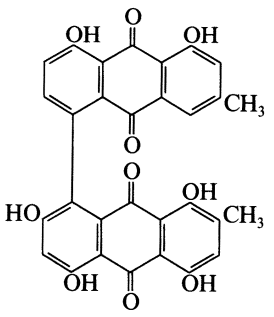
[64381-98-2]

Sjoberg, A.M. *et al*, *J. Chromatogr.*, 1985, **318**, 149 (*hplc, chromatog*)
Takayanagi, M. *et al*, *Appl. Spectrosc.*, 1986, **40**, 1132 (*raman*)
Ballard, J.M. *et al*, *Org. Mass Spectrom.*, 1986, **21**, 575 (*ms*)
Hinckley, D.A. *et al*, *Spectrochim. Acta, Part A*, 1986, **42**, 747 (*uv*)
Wegener, J.W. *et al*, *Chromatographia*, 1987, **24**, 865 (*hplc, uv*)
Chalmers, J.H. *et al*, *J. Chem. Educ.*, 1987, **64**, 969 (*props*)
Ernsting, N.P. *et al*, *Chem. Phys.*, 1988, **122**, 431 (*spectra*)

Rhodoislandin A R-80007

2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-[1,1′-bianthracene]-9,9′,10,10′-tetrone, 9CI. 2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-1,1′-bianthraquinone

[18783-14-7]



$C_{30}H_{18}O_{10}$ M 538.466

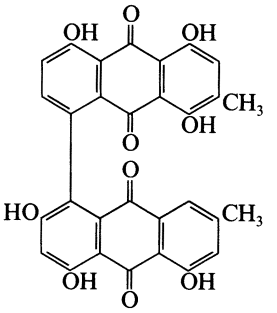
Pigment from *Penicillium islandicum*. Red cryst. Mp >300°.

Ogihara, Y. *et al*, *Tetrahedron Lett.*, 1968, 1881 (*isol, struct, cd, synth*)
Takeda, N. *et al*, *Tetrahedron*, 1973, **29**, 3703 (*bibl*)

Rhodoislandin B R-80008

2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-[1,1′-bianthracene]-9,9′,10,10′-tetrone, 9CI. 2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-1,1′-bianthraquinone

[18693-29-3]



$C_{30}H_{18}O_{10}$ M 538.466

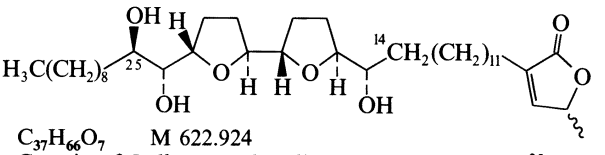
Pigment from *Penicillium islandicum*. Red cryst. Mp >300°.

Ogihara, Y. *et al*, *Tetrahedron Lett.*, 1968, **15**, 1881 (*isol, struct, cd, synth*)
Takeda, N. *et al*, *Tetrahedron*, 1973, **29**, 3703.

Rollinicin R-80009

Updated Entry replacing R-30010

[93303-16-3]



$C_{37}H_{66}O_7$ M 622.924

Constit. of *Rollinia papilionella*. Wax. Mp 30-32°. $[\alpha]_D^{25}$ +6.8° (c, 0.24 in $CHCl_3$).

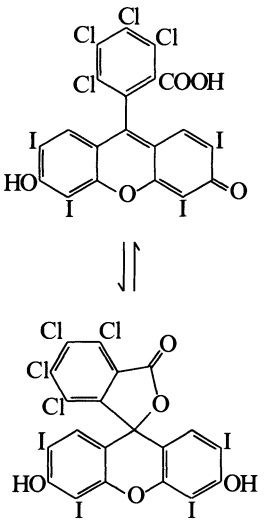
Stereoisomer: [93236-32-9]. ***Isorollinicin***
$C_{37}H_{66}O_7$ M 622.924
From *R. papilionella*. Amorph. Mp 66-68°.

Dabrah, T.T. *et al*, *Phytochemistry*, 1984, **23**, 2013 (*isol*)
Abreo, M.J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 822 (*isol, pmr*)

Rose bengal, 8CI R-80010

4,5,6,7-Tetrachloro-3′,6′-dihydroxy-2′,4′,5′,7′-tetraiodospiro[isobenzofuran-1(3H),9′(9H)xanthen]-3-one, 9CI. 3,4,5,6-Tetrachloro-2′,4′,5′,7′-tetraiodofluorescein, 8CI. CI Solvent red 141

[4159-77-7]



$C_{20}H_4Cl_4I_4O_5$ M 973.677

Singlet-O_2 sensitiser for photooxidations. Dyestuff for cosmetics; food additive. Acid-base indicator. Insol. H_2O. Normally used as di-Na salt.

Di-K salt: [632-68-8]. *Rose Bengal B. CI Acid red 94* Dyestuff for nylon, silk, cellulose materials, inks, cosmetics. Bright bluish pink. Sol. H_2O (blue-red soln., no fluor.).

▷ Possibly teratogenic in rats. Carcinogen. Toxic to freshwater organisms. Binds to and inhibits RNA polymerase.

Lactone-form

Colourless or v. pale pink solid.

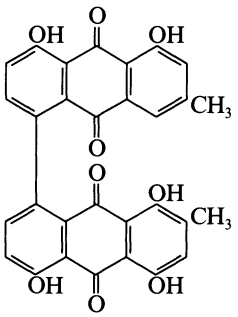
[632-69-9]

Sanders, H.J., *Chem. Eng. News*, 1966, **44**, (42)100, (43)108 (*rev, use*)
Bellin, J.S. *et al*, *J. Chromatogr.*, 1966, **24**, 131 (*chromatog*)
Peeples, W.A. *et al*, *J. Liq. Chromatogr.*, 1981, **4**, 51 (*hplc, purifn*)
Gandin, E. *et al*, *J. Chromatogr.*, 1982, **249**, 393 (*glc, purifn*)
Lamberts, J.J.M. *et al*, *Z. Naturforsch., B*, 1984, **39**, 474 (*uv, use, deriv*)
Lamberts, J.J.M. *et al*, *Tetrahedron*, 1985, **41**, 2183 (*ir, pmr, uv, props, use*)
Ghiggino, K.P. *et al*, *Aust. J. Chem.*, 1988, **41**, 9 (*purifn, uv, props*)

Roseoskyrin R-80011

4,4′,5,5′,8-Pentahydroxy-7,7′-dimethyl-[1,1′-bianthracene]-9,9′,10,10′-tetrone, 9CI. 4,4′,5,5′,8-Pentahydroxy-7,7′-dimethyl-1,1′-bianthraquinone

[18693-27-1]



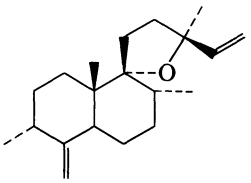
$C_{30}H_{18}O_9$ M 522.467

Pigment from *Penicillium islandicum*. Red cryst. Mp >300°.

Ogihara, Y. *et al*, *Tetrahedron Lett.*, 1968, **15**, 1881 (*isol, struct, cd, synth, pmr*)

Rotalin A R-80012

[119979-81-6]



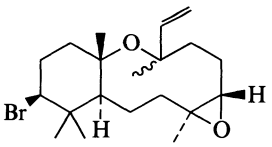
$C_{20}H_{32}O$ M 288.472

Metab. of sponge *Mycale rotalis*. Oil. $[\alpha]_D$ −1.8° (c, 2.8 in $CHCl_3$).

Corriero, G. *et al*, *Tetrahedron*, 1989, **45**, 277.

Rotalin B R-80013

[119979-80-5]

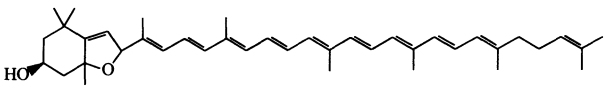


$C_{20}H_{33}BrO_2$ M 385.383

Metab. of sponge *Mycale rotalis*. Amorph. solid. $[\alpha]_D$ +13.9° (c, 0.43 in $CHCl_3$).

Corriero, G. *et al*, *Tetrahedron*, 1989, **45**, 277.

Rubichrome R-80014

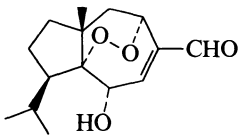


$C_{40}H_{56}O_2$ M 568.881

Isol. from *Tagetes patula* and *Ranunculus acer*. Red-violet platelets ($CHCl_3/Et_2O$). Mp 154°.

Karrer, P. *et al*, *Helv. Chim. Acta*, 1947, **30**, 531.

Rugosal A R-80015

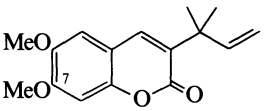


$C_{15}H_{22}O_4$ M 266.336
Constit. of damaged leaves of *Rosa rugosa*. Shows antimicrobial activity. Needles (EtOAc/hexane). Mp 145-147°.

Hashidoko, Y. *et al*, *Phytochemistry*, 1989, **28**, 425.

Rutacultin R-80016

Updated Entry replacing R-00280
3-(1,1-Dimethyl-2-propenyl)-6,7-dimethoxy-2H-1-benzopyran-2-one, 9CI. 3-(1,1-Dimethylallyl)-6,7-dimethoxycoumarin
[31526-60-0]



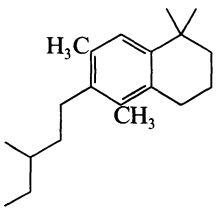
$C_{16}H_{18}O_4$ M 274.316
Constit. of *Ruta graveolens*. Cryst. (pet. ether). Mp 103-104°.

7-O-*De-Me:* [19723-23-0]. ***3-(1,1-Dimethylallyl)scopoletin***
$C_{15}H_{16}O_4$ M 260.289
Constit. of *R. graveolens*. Mp 104-105°.

Steck, W. *et al*, *Phytochemistry*, 1971, **10**, 191 (*isol*)
Ballantyne, M.M. *et al*, *Tetrahedron*, 1971, **27**, 871 (*synth*)
von Brocke, W. *et al*, *Z. Naturforsch.*, *B*, 1971, **26**, 1252 (*deriv*)

Ruzicka's hydrocarbon R-80017

1,2,3,4-Tetrahydro-1,1,5,7-tetramethyl-6-(3-methylpentyl)naphthalene, 9CI
[34418-78-5]

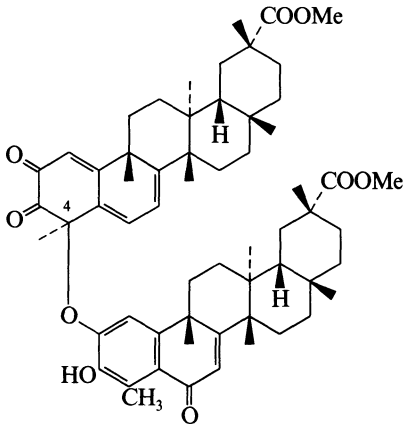


$C_{20}H_{32}$ M 272.473
Liq. $Bp_{0.3}$ 145°. n_D^{25} 1.5220.

Ruzicka, L. *et al*, *Helv. Chim. Acta*, 1931, **14**, 645 (*synth*)
Carman, R.M. *et al*, *Aust. J. Chem.*, 1971, **24**, 1919 (*synth*)
Nasipuri, D. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1973, 1754 (*synth*, *pmr*, *ir*, *uv*)

Rzedowskia bistriterpene R-80018

[121786-61-6]



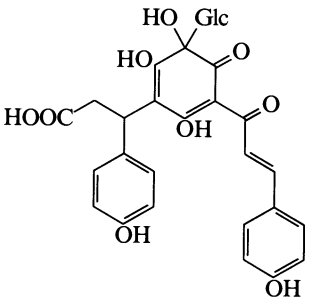
$C_{60}H_{78}O_9$ M 943.271
Compd. not named in the paper. Constit. of roots of *Rzedowskia tolantonguensis*. $[\alpha]_D^{20}$ −143.6° ($CHCl_3$).

4-Epimer: [121688-16-2].
$C_{60}H_{78}O_9$ M 943.271
Constit. of *R. tolantonguensis*. $[\alpha]_D$ +260° ($CHCl_3$). CA name apparently defective.

Gonzalez, A.G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 863.

S

Safflomin C **S-80001**

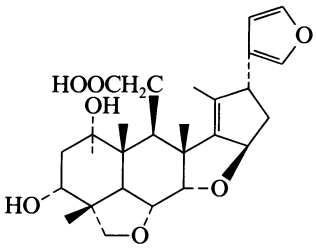


$C_{30}H_{30}O_{14}$ M 614.559
Yellow pigment of Safflower (*Carthamus tinctorius*). Yellow powder. Mp 300° dec.

Ohodera, J. *et al*, *Chem. Lett.*, 1989, 1571.

Salannic acid **S-80002**

Updated Entry replacing S-10003
Nimbidic acid
[29803-85-8]



$C_{26}H_{34}O_7$ M 458.550
Constit. of *Melia dubria*, *M. indica* and *Azadirachta indica*. Cryst. Mp 228-230°.

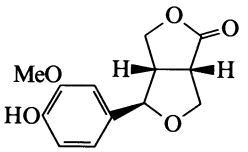
3-O-Ac, 1-O-tigloyl, Me ester: [992-20-1]. *Salannin*
$C_{34}H_{44}O_9$ M 596.716
Minor constit. of nim oil from *M. azadirachta*. Cryst. Mp 167-170°. $[\alpha]_D$ +167° ($CHCl_3$).

1-O-Tigloyl, Me ester:
$C_{32}H_{42}O_8$ M 554.679
From *A. indica*. Cryst. (EtOAc). Mp 214-215°. $[\alpha]_D^{20}$ +134° (c, 1 in $CHCl_3$).

1-(2-Methylbutanoyl), Me ester: Salannol
$C_{32}H_{44}O_8$ M 556.695
From *A. indica*. Cryst. (EtOAc). Mp 208°. $[\alpha]_D^{20}$ +108.7° (c, 1 in $CHCl_3$).

Henderson, R. *et al*, *Tetrahedron*, 1968, **24**, 1525 (*isol, struct*)
de Silva, L.B. *et al*, *Phytochemistry*, 1969, **8**, 1817 (*isol*)
Mitra, C.R. *et al*, *Tetrahedron Lett.*, 1970, 2761 (*struct*)
Nakanishi, K., *Phytochemistry*, 1975, **14**, 283 (*pmr, cmr*)
Kraus, W. *et al*, *Justus Liebigs Ann. Chem.*, 1981, 181 (*isol*)

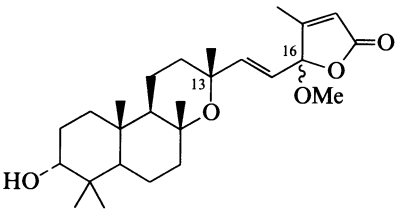
Salicifoliol **S-80003**



$C_{13}H_{14}O_5$ M 250.251
Constit. of *Bupleurum salicifolium*. Cryst. (C_6H_6/pet. ether). Mp 102-103°.

González, A.G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1139 (*isol, pmr, cmr*)

Salviaethiopisolide **S-80004**



$C_{26}H_{40}O_5$ M 432.599
Constit. of *Salvia aethiopis*. Viscous oil. $[\alpha]_D$ +16.25° (c, 0.8 in $CHCl_3$). Mixture of C-16 epimers.

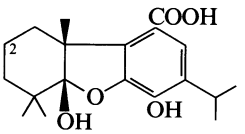
13-Epimer: ***Episalviaethiopisolide***
$C_{26}H_{40}O_5$ M 432.599
Constit. of *S. aethiopis*. Viscous oil. $[\alpha]_D$ +32° (c, 1.53 in $CHCl_3$). Mixt. of C-16 epimers.

[123844-68-8, 123931-55-5, 123931-56-6, 123931-57-7]

Gonzalez, M.S. *et al*, *Tetrahedron*, 1989, **45**, 3575.

Salvicanaric acid **S-80005**

Updated Entry replacing S-70004
[112470-96-9]



$C_{19}H_{26}O_5$ M 334.411
Constit. of *Salvia canariensis*. Foam.

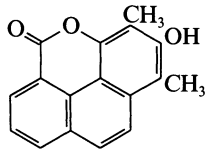
2α-Hydroxy: ***2α-Hydroxysalvicanaric acid***
$C_{19}H_{26}O_6$ M 350.411
Constit. of *S. texana*. Foam.

Gonzalez, A.G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1987, **50**, 341.
Gonzalez, A.G. *et al*, *Tetrahedron*, 1989, **45**, 5203 (*deriv*)

Salvinolactone S-80006

2-Hydroxy-1,3-dimethyl-5H-phenanthro[4,5-bcd]pyran-5-one, 9CI

[120278-21-9]



$C_{17}H_{12}O_3$ M 264.280

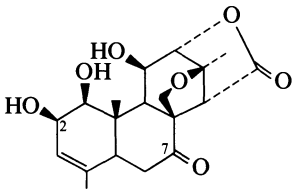
Constit. of *Salvia prionitis*. Cryst. Mp 208-209°.

Lin, L.-Z. *et al*, *Phytochemistry*, 1989, **28**, 177.

Samaderine C S-80007

Updated Entry replacing S-00038

Samaderoside A



$C_{19}H_{24}O_7$ M 364.394

Constit. of *Samadera indica* nuts. Cryst. (EtOAc). Mp 275-276° dec. $[\alpha]_D$ +97.4° (c, 1 in EtOH).

2-Ketone: [803-22-5]. ***Samaderine B***

$C_{19}H_{22}O_7$ M 362.379

Constit. of *S. indica*. Cryst. (EtOAc). Mp 235-240°. $[\alpha]_D$ +67.5° (Py).

7-Alcohol: ***Cedronolin.*** *Cedronylin. 7-Dihydrosamaderine C*

$C_{19}H_{26}O_7$ M 366.410

Isol. from seeds of *S. cedron*. Platelets (MeOH/EtOAc). Mp 263-267° (sinters from 250°). $[\alpha]_D$ +17.2° (c, 0.7 in Py).

2-Ketone, 7-alcohol: ***Cedronin.*** *7-Dihydrosamaderine B*

$C_{19}H_{24}O_7$ M 364.394

Isol. from seeds of *S. sedron*. Needles (MeOH). Mp 275-280° (sinters from 240°). $[\alpha]_D$ −12.6° (c, 0.714 in Py).

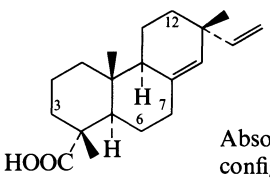
Zylber, J. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 2016.

Sandaracopimaric acid S-80008

Updated Entry replacing S-00067

Cryptopimaric acid. 8(14),15-Isopimaradien-18-oic acid

[471-74-9]



Absolute configurtion

$C_{20}H_{30}O_2$ M 302.456

Constit. of *Pinus*, *Juniperus* and *Cupressus* spp. Also from *Cryptomera japonica*, *Tetraclinis articulata*, *Callitris* sp. and *Agathus australis*. Cryst. (MeOH aq.). Mp 171-173° (softens at 163°). $[\alpha]_D$ −20° (c, 2.6 in $CHCl_3$).

3β-Hydroxy: [35951-45-2]. *3β-Hydroxyisopimara-8(14),15-dien-18-oic acid. 3β-Hydroxysandaracopimaric acid*

$C_{20}H_{30}O_3$ M 318.455

Constit. of *J. rigida*. Cryst. Mp 261°. $[\alpha]_D$+ ±0° (Py).

6α-Hydroxy: [19907-23-4]. *6α-Hydroxyisopimara-8(14),15-dien-18-oic acid. 6α-Hydroxysandaracopimaric acid*

$C_{20}H_{30}O_3$ M 318.455

Constit. of *J. phoenicea*. Cryst. (Me_2CO). Mp 265-267°.

7α-Hydroxy: 7α-Hydroxyisopimara-8(14)15-dien-18-oic acid. 7α-Hydroxysandaracopimaric acid

$C_{20}H_{30}O_3$ M 318.455

Constit. of *J. communis*. Oil (as Me ester). $[\alpha]_D$ −41° (c, 0.8 in $CHCl_3$) (Me ester).

12β-Hydroxy: [1235-75-2]. *12β-Hydroxyisopimara-8(14),15-dien-18-oic acid. 12β-Hydroxysandaracopimaric acid*

$C_{20}H_{30}O_3$ M 318.455

Isol. from *Callitris quadrivalvis*. Needles (Me_2CO). Mp 269-270°. $[\alpha]_D$ −11° (c, 0.4 in EtOH).

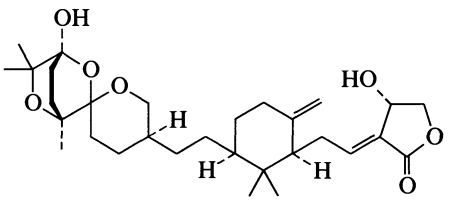
12β-Acetoxy: 12β-Acetoxyisopimara-8(14),15-dien-18-oic acid. 12β-Acetoxysandaracopimaric acid

$C_{22}H_{32}O_4$ M 360.492

Constit. of *Tetraclinis articulata*. Cryst. Mp 140.5-141.5°, Mp 156-158.5°, Mp 170° (trimorph.). $[\alpha]_D$ −50° (EtOH).

Edwards, O.E. *et al*, *Can. J. Chem.*, 1960, **38**, 663 (*isol, struct*)
Arya, V.P. *et al*, *Acta Chem. Scand.*, 1961, **15**, 682 (*struct*)
Bose, A.K. *et al*, *Chem. Ind. (London)*, 1963, 254 (*abs config*)
Enzell, C. *et al*, *Ark. Kemi*, 1965, **23**, 367 (*ms*)
ApSimon, J.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 361 (*pmr*)
Joye, N.M. *et al*, *J. Org. Chem.*, 1966, **31**, 320 (*isol*)
Afonso, A., *J. Am. Chem. Soc.*, 1968, **90**, 7375 (*synth*)
Tabacik, C. *et al*, *Phytochemistry*, 1971, **10**, 2147 (*6α-Hydroxysandaracopimaric acid*)
Lapasset, J. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 3321 (*12β-Hydroxysandaracopimaric acid*)
Wenkert, E. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 4367 (*cmr*)
Kozo, D. *et al*, *Phytochemistry*, 1972, **11**, 841 (*3β-Hydroxysandaracopimaric acid*)
de Pascual Teresa, J. *et al*, *Phytochemistry*, 1980, **19**, 1153 (*7α-Hydroxysandaracopimaric acid*)

Saponaceolide A S-80009



$C_{30}H_{46}O_7$ M 518.689

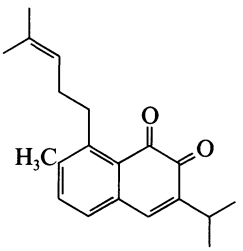
Prod. by *Tricholoma saponaceum*. Cytotoxic agent. Needles (Me_2CO/hexane). Mp 145-146°. $[\alpha]_D^{20}$ +78.14° (c, 1.1 in $CHCl_3$).

De Bernardi, M. *et al*, *Tetrahedron*, 1988, **44**, 235 (*isol, struct*)

Saprorthoquinone S-80010

7-Methyl-3-(1-methylethyl)-8-(4-methyl-3-pentenyl)-1,2-naphthalenedione, 9CI. 3-Isopropyl-7-methyl-8-(4-methyl-3-pentenyl)-1,2-naphthoquione

[102607-41-0]

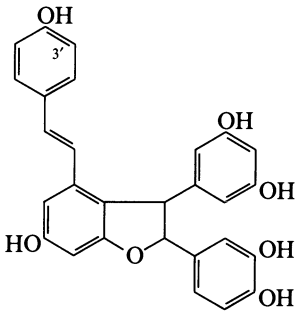


$C_{20}H_{24}O_2$ M 296.408
Constit. of *Salvia prionitis*. Cryst. Mp 97-98°. A 4,5-seco-5,10-friedoabietane.

Simoes, F. *et al*, *Phytochemistry*, 1986, **25**, 755 (*synth*)
Lin, L.-Z. *et al*, *Phytochemistry*, 1989, **28**, 177 (*isol*)

Scirpusin A S-80011

Updated Entry replacing S-50031
[69297-51-4]

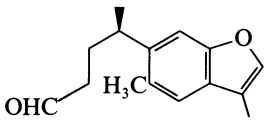


$C_{28}H_{22}O_7$ M 470.478
Constit. of *Scirpus fluviatilis* and *S. maritimus*. Pale brown amorph. powder.

3'-Hydroxy: [69297-49-0]. ***Scirpusin B***
$C_{28}H_{22}O_8$ M 486.477
Constit. of *S. fluviatilis* and *S. maritimus*. Pale brown amorph. powder.

Nakajima, K. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 3050 (*isol*)
Powell, R.G. *et al*, *J. Nat. Prod.* (*Lloydia*), 1987, **50**, 293 (*isol*)

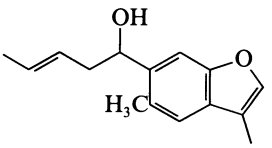
Secoeurabicanal S-80012



$C_{15}H_{18}O_2$ M 230.306
Constit. of *Euryops arabicus*. A seco-furoeremophilane.

Hafez, S. *et al*, *Phytochemistry*, 1989, **28**, 843.

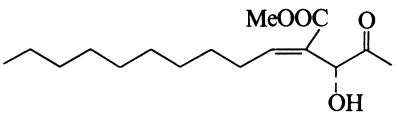
Secoeurabicol S-80013



$C_{15}H_{18}O_2$ M 230.306
Constit. of *Euryops arabicus*. A seco-furoeremophilane.

Hafez, S. *et al*, *Phytochemistry*, 1989, **28**, 843.

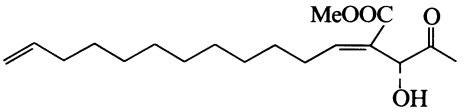
Secoisolancifolide S-80014



$C_{16}H_{28}O_4$ M 284.395
(R)-form
Constit. of *Actinodaphne longifolia*. Oil. $[\alpha]_D$ +102.7° (c, 0.49 in $CHCl_3$).

Tanaka, H. *et al*, *Phytochemistry*, 1989, **28**, 1905.

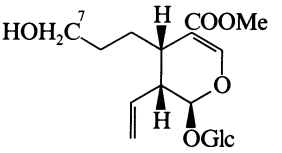
Secoisoobtusilactone S-80015



$C_{18}H_{30}O_4$ M 310.433
(R)-form
Constit. of *Actinodaphne longifolia*. Oil. $[\alpha]_D$ +72.2° (c, 0.18 in $CHCl_3$).

Tanaka, H. *et al*, *Phytochemistry*, 1989, **28**, 1905.

Secologanol S-80016



$C_{17}H_{26}O_{10}$ M 390.386
Constit. of *Gentiana verna*.

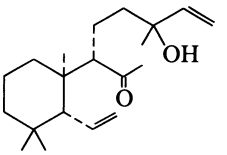
7-Ac: 7-Acetylsecologanol
$C_{19}H_{28}O_{11}$ M 432.424
Constit. of *G. verna*.

7-(2,5-Dihydroxybenzoyl):
$C_{24}H_{30}O_{13}$ M 526.493
Constit. of *G. verna*.

Mpondo, E.M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1146 (*isol*, *pmr*, *cmr*)

Secomanool S-80017

[118855-41-7]

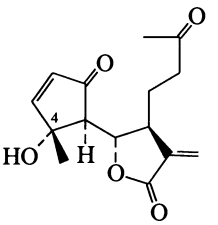


$C_{20}H_{34}O_2$ M 306.487
Constit. of *Fleischmannia microstemon*. Oil. $[\alpha]_D^{24}$ −15° (c, 1.2 in $CHCl_3$). A 7,8-secolabdane.

Tamayo-Castillo, G. *et al*, *Phytochemistry*, 1988, **27**, 3322.

Secotanapartholide A S-80018

seco-*Tanapartholide A*
[103063-09-8]

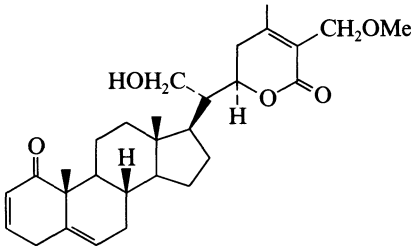


$C_{15}H_{18}O_5$ M 278.304
Constit. of *Tanacetum parthenium*. Oil. $[\alpha]_D^{20}$ −11.2° (c, 1.05 in EtOH).

4-Epimer: [85758-26-5]. ***Secotanapartholide B.*** seco-*Tanapartholide B*
$C_{15}H_{18}O_5$ M 278.304
Constit. *T. parthenium*. Oil.

Begley, M.J. *et al*, *Phytochemistry*, 1989, **28**, 940.

Secowithametelin S-80019

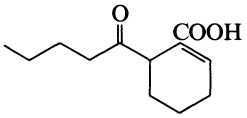


$C_{29}H_{40}O_5$ M 468.632
Constit. of *Datura metel*. Plates (EtOAc/pet. ether). Mp 190°. $[\alpha]_D$ +28.53° (c, 0.75 in $CHCl_3$).

Kundu, S. *et al*, *Phytochemistry*, 1989, **28**, 1769.

Sedanonic acid S-80020

6-(1-Oxopentyl)-1-cyclohexene-1-carboxylic acid, 9CI
[6697-07-0]



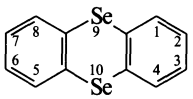
$C_{12}H_{18}O_3$ M 210.272
Isol. from celery oil (*Apium graveolens*) after hydrol., and from roots of *Cnidium officinale*. Cryst. (C_6H_6). Mp 113°.

[62006-38-6]

Ciamician, G. *et al*, *Ber.*, 1897, **30**, 492, 501, 1419 (*isol, struct*)
Barton, D.H.R. *et al*, *J. Chem. Soc.*, 1963, 1916 (*isol*)
Bjeldanes, L.F. *et al*, *J. Org. Chem.*, 1977, **42**, 2333 (*ir, pmr, ms*)

Selenanthrene, 9CI S-80021

[262-30-6]



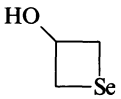
$C_{12}H_8Se_2$ M 310.115
Needles or prisms. Mp 180-181°.

9,10-Dioxide:
$C_{12}H_8O_2Se_2$ M 342.114
Mp 270°.

Krafft, F. *et al*, *Ber.*, 1896, **29**, 443 (*synth*)
Cullinane, N.M. *et al*, *J. Chem. Soc.*, 1939, 151 (*synth*)

3-Selenetanol S-80022

3-Hydroxyselenetane
[73903-64-7]



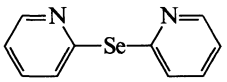
C_3H_6OSe M 137.040
$Bp_{3.5}$ 80-85°, $Bp_{0.8}$ 60-62°.

Ac: [112422-93-2].
$C_5H_8O_2Se$ M 179.077
Yellow oil. Dec. on dist.

Arnold, A.P. *et al*, *Aust. J. Chem.*, 1983, **36**, 815 (*synth, pmr*)
Polson, G. *et al*, *J. Org. Chem.*, 1988, **53**, 791 (*synth, pmr, cmr, ms*)

2,2′-Selenobispyridine, 9CI S-80023

2,2′-Selenodipyridine. 2,2′-Dipyridyl selenide
[66491-49-4]



$C_{10}H_8N_2Se$ M 235.147
Yellow oil. $Bp_{0.5}$ 135-140°.

B, 2HBr: [66491-50-7].
Cryst. + $\frac{1}{2}H_2O$. Mp 224-226° dec.

Grant, H.G. *et al*, *Z. Naturforsch.*, *B*, 1978, **33**, 118 (*synth, uv*)
Keats, N.G. *et al*, *J. Heterocycl. Chem.*, 1979, **16**, 1369 (*ms*)
Pierini, A.B. *et al*, *J. Org. Chem.*, 1984, **49**, 486 (*synth, pmr*)
Summers, L.A., *J. Heterocycl. Chem.*, 1987, **24**, 533 (*rev, bibl*)

4,4′-Selenobispyridine, 9CI S-80024

4,4′-Selenodipyridine. 4,4′-Dipyridyl selenide
[87385-48-6]

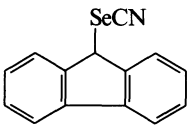
Has bactericidal and herbicidal props. Needles. Mp 63-65°.

B, 2HCl: Needles (EtOH/EtOAc). Mp 225-230°.

Jerchel, D. *et al*, *Chem. Ber.*, 1956, **89**, 2921 (*synth*)
Boduszek, B. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1983, **57**, 641 (*synth, ir, ms, pmr*)
Summers, L.A., *J. Heterocycl. Chem.*, 1987, **24**, 533 (*bibl*)

9-(Selenocyanato)fluorene S-80025

[114263-69-3]

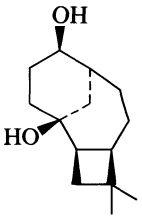


$C_{14}H_9NSe$ M 270.192
Pale yellow powder. Mp 109-111°.

Meinke, P.T. *et al*, *J. Org. Chem.*, 1988, **53**, 3632 (*synth, pmr, cmr, ir, ms*)

Senecrassidiol S-80026

Updated Entry replacing S-00284



$C_{15}H_{26}O_2$ M 238.369
Constit. of *Senecio crassissimus*. Cryst. (2-propanol). Mp 93-96°. $[\alpha]_D^{24}$ −10.9° (c, 0.23 in $CHCl_3$).

5-Deoxy, 6-oxo:
$C_{15}H_{24}O_2$ M 236.353
Constit. of *Eurypon* sp. Oil. $[\alpha]_D$ −3.3° (c, 0.9 in $CHCl_3$).

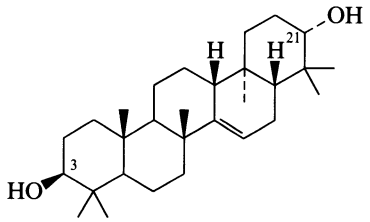
5-Deoxy, 6-oxo, 8-Me ether:
$C_{16}H_{26}O_2$ M 250.380
Constit. of a *E.* sp. Oil. $[\alpha]_D$ −5.6° (c, 0.9 in $CHCl_3$).

6α-Hydroxy, 6,8-dideoxy, 7,8-didehydro:
$C_{15}H_{24}O$ M 220.354
Constit. of a *E.* sp. Oil. $[\alpha]_D$ −12.8° (c, 0.9 in $CHCl_3$).

Bohlmann, F. *et al*, *Phytochemistry*, 1981, **20**, 469.
Barrow, C.J. *et al*, *Aust. J. Chem.*, 1988, **41**, 1755 (*derivs*)

14-Serratene-3,21-diol S-80027

Updated Entry replacing S-10033



(3β,21α)-*form*

$C_{30}H_{50}O_2$ M 442.724

(3β,21α)-form [2239-24-9] ***Pinusenediol.*** *Serratenediol*
Constit. of the club moss *Lycopodium serratum* and *Pinus* spp. Cryst. (EtOH). Mp 302.5-304.5°. $[\alpha]_D^{22}$ −19° (c, 0.9 in $CHCl_3$).

3-Me ether: 3β-Methoxy-14-serraten-21α-ol
$C_{31}H_{52}O_2$ M 456.751
Constit. of sugar pine (*P. lambertiana*). Cryst. (EtOH). Mp 319-322.5°. $[\alpha]_D^{22}$ −5° ($CHCl_3$).

Di-Me ether: 3β,21α-Dimethoxy-14-serratene
$C_{32}H_{54}O_2$ M 470.777
Constit. of *P. lambertiana*. Cryst. (EtOH). Mp 320.5-323.5°. $[\alpha]_D^{22}$ +21° ($CHCl_3$).

3-O-α-L-Arabinopyranosyl: [80235-56-9]. ***Inundoside* A**
$C_{36}H_{60}O_7$ M 604.866
Constit. of *L. inundatum*. Needles ($CHCl_3$/MeOH). Mp >300°.

21-Ac, 3-O-α-L-arabinopyranosyl: [80235-55-8]. ***Inundoside B***
$C_{38}H_{62}O_8$ M 646.903
Constit. of *L. inundatum*. Needles (MeOH). Mp >300°.

3-O-(4-O-p-Coumaroyl-α-L-arabinopyranosyl): [80242-62-2]. ***Inundoside*** D_1
$C_{45}H_{66}O_9$ M 751.011
Constit. of *L. inundatum*. Needles ($CHCl_3$/MeOH). Mp 286-290°.

21-Ac, 3-O-(4-O-p-coumaroyl-α-L-arabinopyranosyl): [80235-53-6]. ***Inundoside*** D_2
$C_{47}H_{68}O_{10}$ M 793.048
Constit. of *L. inundatum*. Needles ($CHCl_3$/MeOH). Mp >300°.

3-Ac: Serratenediol 3-monoacetate
$C_{32}H_{52}O_3$ M 484.761
Isol. from *L. serratum*. Mp 319-320°. $[\alpha]_D^{10}$ −5.7° (c, 1.06 in $CHCl_3$).

(3β,21β)-form [1449-06-5]
21-epi-*Serratenediol*
Constit. of club moss *L. serratum* and the bark of the sugar pine. Cryst. (EtOH). Mp 303-308°. $[\alpha]_D^{23}$ −19° (c, 1.29 in $CHCl_3$).

3-Me ether: [19902-59-1]. *3β-Methoxy-14-serraten-21β-ol*
$C_{31}H_{52}O_2$ M 456.751
Constit. of the bark of *Picea sitchensis*. Cryst. (EtOH). Mp 307-308°. $[\alpha]_D$ +3° ($CHCl_3$).

21-Me ether: [24433-28-1]. *21β-Methoxy-14-serraten-3β-ol*
$C_{31}H_{52}O_2$ M 456.751
Constit. of the bark of *Pinus contorta*. Cryst. (CH_2Cl_2/MeOH). Mp 250.5-252°. $[\alpha]_D^{21}$ −43.5° (c, 0.9 in $CHCl_3$).

3-O-α-L-Arabinopyranosyl: [80244-83-3]. ***Inundoside E***
$C_{36}H_{60}O_7$ M 604.866
Constit. of *L. inundatum*. Needles ($CHCl_3$/MeOH). Mp >300°.

3-O-(4-O-p-Coumaroyl-α-L-arabinopyranosyl): [80235-52-5]. ***Inundoside F***
$C_{45}H_{66}O_9$ M 751.011
Constit. of *L. inundatum*. Needles ($CHCl_3$/MeOH). Mp >300°.

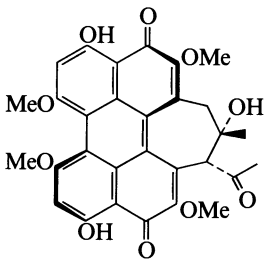
(3α,21β)-form
diepi-*Serratenediol. Diepiserratenediol*
Minor constit. of *Pinus banksiana* bark. Cryst. (EtOH). Mp 300-301°. $[\alpha]_D^{23}$ −32° (c, 0.9 in $CHCl_3$).

3-Me ether: [19902-63-7]. *3α-Methoxy-14-serraten-21β-ol*
$C_{31}H_{52}O_2$ M 456.751
Isol. from *Pinus sitchensis* and *P. abies*. Cryst. (EtOH). Mp 276-277°. $[\alpha]_D^{20}$ −55° ($CHCl_3$).

Di-Me ether: [28161-29-7]. *3β,21β-Dimethoxy-14-serratene*
$C_{32}H_{54}O_2$ M 470.777
From *P. sitchensis*. Cryst. by subl. Mp 254-256°.

Rowe, J.W. *et al, Tetrahedron Lett.*, 1964, 2347; 1965, 2745 (*isol, struct*)
Inubushi, Y. *et al, Chem. Pharm. Bull.*, 1965, **13**, 104 (*isol, struct*)
Kutney, J.P. *et al, Tetrahedron*, 1969, **25**, 3731 (*isol*)
Roners, J.H. *et al, Can. J. Chem.*, 1970, **48**, 1021 (*isol*)
Rowe, J.W. *et al, Phytochemistry*, 1972, **11**, 365 (*isol*)
Tsuda, Y. *et al, Chem. Pharm. Bull.*, 1981, **29**, 2123 (*struct*)
Tsuda, Y. *et al, Chem. Pharm. Bull.*, 1982, **30**, 1500 (*synth*)

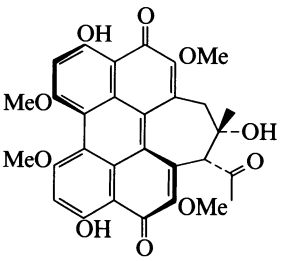
Shiraiachrome A S-80028



$C_{30}H_{26}O_{10}$ M 546.529
Pigment from *Shiraia bambusicola*. Deep red cryst. Mp 247-250°.

Wu, H., *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 948 (*isol, pmr, cmr*)

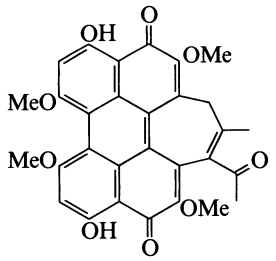
Shiraiachrome B S-80029



$C_{30}H_{26}O_{10}$ M 546.529
Constit. of *Shiraia bambusicola*. Deep red cryst. Mp 247-248°.

Wu, H. *et al, J. Nat. Prod.* (*Lloydia*), 1989, **52**, 949 (*isol, pmr*)

Shiraiachrome C S-80030



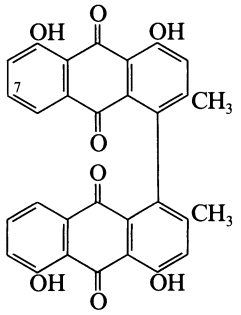
$C_{30}H_{24}O_9$ M 528.514
Constit. of *Shiraia bambusicola*. Red cryst. Mp 278-280°.

Wu, H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 948 (*isol, pmr*)

Siameanin S-80031

4,4′,5,5′-Tetrahydroxy-2,2′-dimethyl-[1,1′-bianthracene]-9,9′,10′,10′-tetrone, 9CI. 4,4′,5,5′-Tetrahydroxy-2,2′-dimethyl-1,1′-bianthraquinone. 4,4′-Bi[1,8-Dihydroxy-3-methylanthraquinone]. 4,4′-Bichrysophanol

[13993-55-0]



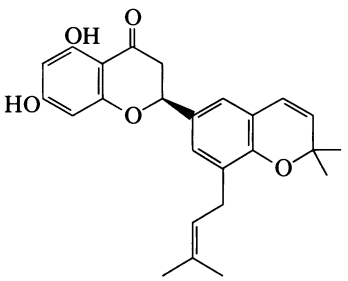
$C_{30}H_{18}O_8$ M 506.467
Isol. from peel of *Cassia siamea* and from leaves of *C. occidentalis*. Red microneedles (C_6H_6/EtOAc). Mp 323-325° dec.

Tetra-Ac: Mp 170°.

7-Hydroxy: ***Cassianin***
$C_{30}H_{18}O_9$ M 522.467
Isol. from *C. siamea*. Orange-red needles (C_6H_6/EtOAc). Mp 350-360° dec.

Chatterjee, A. *et al*, *J. Indian Chem. Soc.*, 1964, **41**, 415 (*isol, uv, ir, pmr, struct*)
Tiwari, R.D. *et al*, *Planta Med.*, 1977, **32**, 375 (*isol*)

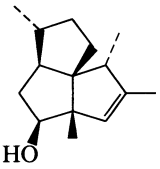
Sigmoidin E S-80032



$C_{25}H_{26}O_5$ M 406.477
(***S***)-***form*** [116174-67-5]
Constit. of *Erythrina sigmoidea*. $[\alpha]_D$ −36.8° (c, 1.36 in MeOH).

Promsattha, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 611.

5-Silphiperfolen-3-ol S-80033

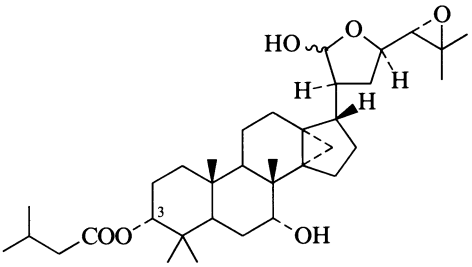


$C_{15}H_{24}O$ M 220.354
Constit. of *Artemisia laciniata*. Oil.

Brendel, J. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2371 (*synth*)

Skimmearepin A S-80034

[118156-16-4]



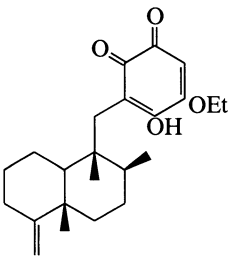
$C_{35}H_{56}O_6$ M 572.824
Constit. of *Skimmia japonica*. Shows insect antifeedant activity. Cryst. (EtOH). Mp 164.5-165.5°. $[\alpha]_D^{20}$ −22.7° (c, 0.2 in EtOH).

3-Deacyl, 3-(2Z,4E,6E-decatrienoyl): [118156-15-3].
Skimmiarepin B
$C_{40}H_{60}O_6$ M 636.910
Constit. of *S. japonica*. Shows insect antifeedant activity. Cryst. (Me_2CO). Mp 168-169°. $[\alpha]_D^{18}$ −39.8° (c, 0.11 in $CHCl_3$).

Ochi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3225.

Smenorthoquinone S-80035

[121994-49-8]

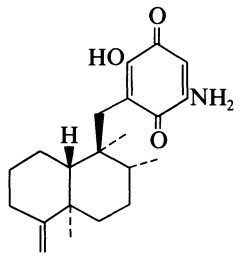


$C_{23}H_{32}O_4$ M 372.503
Constit. of *Smenospongia* sp. Antimicrobial and cytotoxic. Yellow needles (MeOH).

Kondracki, M.-L. *et al*, *Tetrahedron*, 1989, **45**, 1995.

Smenospongine S-80036

Updated Entry replacing S-60036



$C_{21}H_{29}NO_3$ M 343.465

Quinoterpenoid antibiotic. Prod. by the sponge *Smenospongia* sp. Cytotoxic and antimicrobial agent. Red cryst. Mp 153-155°.

N-(2-phenylethyl): ***Smenospongidine***
$C_{29}H_{37}NO_3$ M 447.616
Constit. of *S.* sp. Antimicrobial and cytotoxic. Cryst. (MeOH). Mp 168-170°.

N-(3-methylbutyl): ***Smenospongianine***
$C_{26}H_{39}NO_3$ M 413.599
Constit. of *S.* sp. Antimicrobial and cytotoxic. Cryst. Mp 170-172°.

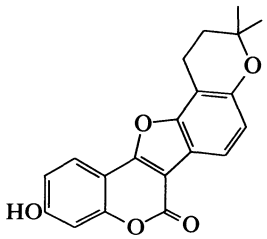
N-(2-methylpropyl): ***Smenospongorine***
$C_{25}H_{37}NO_3$ M 399.572
Constit. of *S* sp. Antimicrobial and cytotoxic.

Kondracki, M.-L. *et al*, *Tetrahedron*, 1989, **45**, 1995.

Sojagol S-80037

*2,3-Dihydro-10-hydroxy-3,3-dimethyl-1*H,*7*H-*furo[2,3-*c*:5,4-f′]bis[1]benzopyran-7-one, 9CI. Soyagol*

[18979-00-5]



$C_{20}H_{16}O_5$ M 336.343

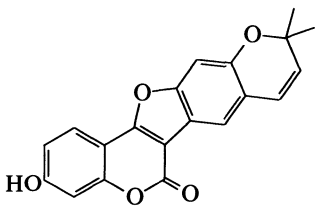
Phytoalexin from leaves and hypocotyls of *Glycine max* and from mung beans (*Phaseolus aureus*). Needles by subl. Mp 284-286°.

Zilg, H. *et al*, *Phytochemistry*, 1968, **7**, 1765 (*isol, ir, ms, struct*)
Keen, N.T. *et al*, *Phytochemistry*, 1972, **11**, 1031 (*isol, uv*)

Sophoracoumestan A S-80038

*3-Hydroxy-10,10-dimethyl-6*H,*10*H-*furo[3,2-*c*:4,5-g′]bis[1]benzopyran-6-one, 9CI*

[77369-93-8]



$C_{20}H_{14}O_5$ M 334.328

Isol. from roots of *Sophora franchetiana*. Needles (MeOH). Mp >300°.

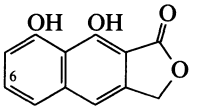
Komatsu, M. *et al*, *Chem. Pharm. Bull.*, 1981, **29**, 532 (*isol, uv, ms, pmr, struct*)

β-Sorigenin S-80039

Updated Entry replacing D-04767

*8,9-Dihydroxynaphtho[2,3-*c*]furan-1(3*H*)-one, 9CI. Sorigenin*

[492-23-9]



$C_{12}H_8O_4$ M 216.193

Pale-yellow cryst. Mp 237-240°.

Di-Ac: Cryst. Mp 229-230°.

8-O-β-D-Primeveroside: [519-99-3]. ***β-Sorinin***
$C_{23}H_{26}O_{13}$ M 510.451
Isol. from bark of *Rhamnus japonica*. Amorph. powder.

Di-Me ether: [63744-12-7].
Pale-yellow cryst. (Me_2CO/hexane). Mp 174.5-176°.

6-Methoxy: ***α-Sorigenin***
$C_{13}H_{10}O_5$ M 246.219
From *R. japonica*. Yellowish needles (EtOH). Mp 227-229° dec. (185°).

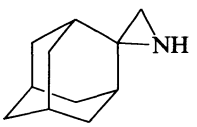
6-Methoxy, 8-O-β-D-primeveroside: ***α-Sorinin***
$C_{24}H_{28}O_{14}$ M 540.477
Isol. from *R. japonica*. Needles or prisms (EtOH aq.). Mp 159°.

Haber, R.G. *et al*, *Helv. Chim. Acta*, 1956, **39**, 1654 (*struct, synth*)
Matsui, M. *et al*, *Agric. Biol. Chem.*, 1962, **27**, 40 (*synth*)
Horii, Z. *et al*, *Chem. Pharm. Bull.*, 1963, **11**, 312, 317 (*struct, synth*)
Hauser, F.M. *et al*, *J. Org. Chem.*, 1977, **42**, 4155 (*synth*)

Spiro[aziridine-2,2′-tricyclo[3.1.1.1^{3,7}]decane], 9CI S-80040

Spiro[adamantane-2,2′-aziridine]

[59591-91-2]



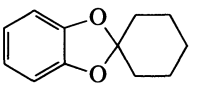
$C_{11}H_{17}N$ M 163.262

Mp 141-143°.

Sasaki, T. *et al*, *Tetrahedron*, 1976, **32**, 437.

Spiro[1,3-benzodioxole-2,1′-cyclohexane] S-80041

[182-55-8]

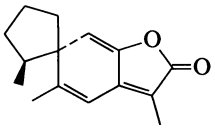


$C_{12}H_{14}O_2$ M 190.241

Mp 51-52° (47°).

Birch, A.J., *J. Chem. Soc.*, 1947, 102 (*synth*)
Antus, S. *et al*, *Chem. Ber.*, 1989, **122**, 1017 (*synth, pmr*)

Spiroeuryolide S-80042

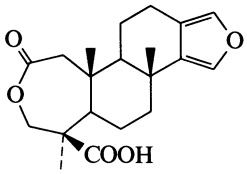


$C_{15}H_{18}O_2$ M 230.306
Constit. of *Euryops arabicus*.

Hafez, S. *et al*, *Phytochemistry*, 1989, **28**, 843.

Spongialactone A S-80043

[120030-04-8]

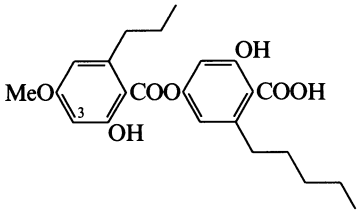


$C_{20}H_{26}O_5$ M 346.422
Constit. of *Spongia arabica*. Amorph. powder.

Hirsch, S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 1243 (*isol, pmr, cmr*)

Stenosporic acid S-80044

Updated Entry replacing S-00765
2-Hydroxy-4-[(2-hydroxy-4-methoxy-6-propylbenzoyloxy)]-6-pentylbenzoic acid, 9CI
[27240-56-8]



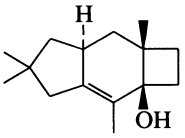
$C_{23}H_{28}O_7$ M 416.470
Isol. from *Ramalina stenospora*, *Nephroma cellulosum* and *Pertusaria* spp. Cryst. (cyclohexane). Mp 112-114°.

Me ester: Cryst. (hexane). Mp 35-36°.

3-Chloro: [120091-96-5]. ***3-Chlorostenosporic acid***
$C_{23}H_{27}ClO_7$ M 450.915
Constit. of *Dimelaena* cf. *californica*. Cryst. (CH_2Cl_2/pet. ether). Mp 138°.

Culberson, C.F., *Phytochemistry*, 1970, **9**, 841 (*isol, synth*)
Culberson, C.F. *et al*, *Bryologist*, 1972, **75**, 362 (*isol*)
Elix, J.A., *Aust. J. Chem.*, 1974, **27**, 1767 (*synth*)
Renner, B. *et al*, *Z. Naturforsch.*, *C*, 1978, **33**, 340 (*isol*)
Elix, J.A. *et al*, *Aust. J. Chem.*, 1988, **41**, 1789 (*isol, synth, deriv*)

3-Sterpurenol S-80045

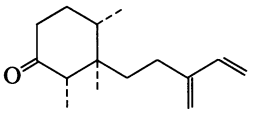


$C_{15}H_{24}O$ M 220.354
Ac: ***3-Acetoxysterpurene***
$C_{17}H_{26}O_2$ M 262.391

Metab. of *Alcyonum acaule*. Oil. $[\alpha]_D$ +128.6° (c, 2.2 in $CHCl_3$).

Cimino, G. *et al*, *Tetrahedron*, 1989, **45**, 6479.

Striatenone S-80046

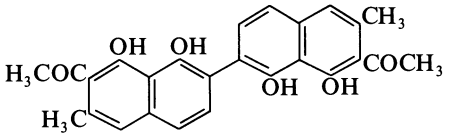


$C_{15}H_{24}O$ M 220.354
Constit. of *Porella navicularis*. Oil. $[\alpha]_D$ −9.1° (c, 0.11 in $CHCl_3$).

Toyota, M. *et al*, *Phytochemistry*, 1989, **28**, 1661.

Stypandrol S-80047

Updated Entry replacing S-50130
7,7′-Diacetyl-1,1′,8,8′-tetrahydroxy-6,6′-dimethyl-2,2′-binaphthyl. Hemerocallin
[99305-33-6]

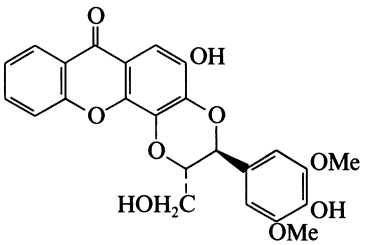


$C_{26}H_{22}O_6$ M 430.456
Constit. of *Stypandra imbricata*, *Dianella revoluta* and *Hemerocallis* spp. Shows neurotoxic properties. Orange needles ($CHCl_3$). Mp 265-266° dec.

Colegate, S.M. *et al*, *Aust. J. Chem.*, 1985, **38**, 1233 (*isol*)
Wang, J.-H. *et al*, *Phytochemistry*, 1989, **28**, 1825 (*pmr, cmr, struct*)

Subalatin S-80048

[119269-69-1]

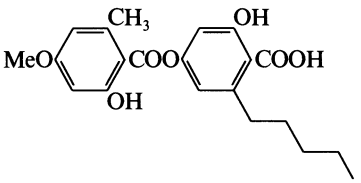


$C_{24}H_{20}O_9$ M 452.417
Constit. of *Hypericum subalatum*. Pale yellow needles ($CHCl_3$/MeOH). Mp 265° dec. $[\alpha]_D^{25}$ +600° (c, 0.005 in MeOH).

Chen, M.-T., *Heterocycles*, 1988, **27**, 2589.

Subsphaeric acid S-80049

[120091-90-9]



$C_{21}H_{24}O_7$ M 388.416

Constit. of *Dimelaena thysanota*. Cryst. (EtOAc/pet. ether). Mp 120°.

Elix, J.A. *et al*, *Aust. J. Chem.*, 1988, **41**, 1789 (*isol, struct, synth*)

Sulfoacetic acid S-80050

Sulfoethanoic acid

[123-43-3]

$HOOCCH_2SO_3H$

$C_2H_4O_5S$ M 140.117

Reagent for Liebermann-Burchard colorimetric test for steroids. Reaction catalyst. Hygroscopic cryst. + $1H_2O$ (H_2O). Mp 84-86°. Bp 245° dec.

Py salt: [21372-73-6]. Mp 151-152°.

Carboxy-Et ester: $C_4H_8O_5S$ M 168.170 Mp 175° (as K salt).

Di-Et ester: $C_6H_{12}O_3S$ M 164.225 $Bp_{0.5}$ 116°.

Dianilide: $C_{14}H_{14}N_2O_3S$ M 290.342 Mp 150-151°.

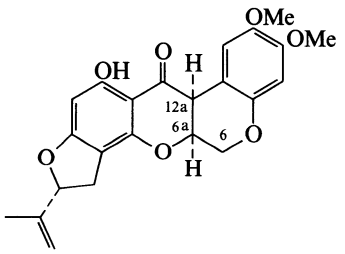
[5462-60-2, 16697-66-8, 22128-42-3, 64707-21-7]

Folkers, K. *et al*, *J. Am. Chem. Soc.*, 1944, **66**, 1083 (*synth*)
Lehmann, J. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 4469.
Hoogenboom, B.E. *et al*, *J. Org. Chem.*, 1969, **34**, 3414 (*deriv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 7.
Mao, J.C.H. *et al*, *Antimicrob. Agents Chemother.*, 1985, **27**, 197.

Sumatrol S-80051

Updated Entry replacing S-01008

[82-10-0]



$C_{23}H_{22}O_7$ M 410.423

Isol. from *Crotalaria burhia, Derris malaccensis, Millettia auriculata, Piscidia erythrina* and *Tephrosia toxicaria*. Needles (EtOH or Me_2CO). Spar. sol. dil. NaOH. Mp 174.5-177.5° (183-194°, 195-196°). $[\alpha]_D$ −184° (c, 1.335 in C_6H_6).

Ac: Mp 218-219°. $[\alpha]_D$ +57° (C_6H_6), −20.5° (Me_2CO).

Oxime: Needles (EtOH aq.). Mp 245-247°.

6α-Hydroxy: [65160-15-8]. ***Villosin.*** *6-Hydroxysumatrol* $C_{23}H_{22}O_8$ M 426.422 Constit. of the pods of *T. villosa*. Mp 133°.

6-Oxo: [65160-16-9]. ***Villosone*** $C_{23}H_{18}O_8$ M 422.390 Constit. of *T. villosa*. Mp 268°.

6α-Methoxy: [65160-17-0]. ***Villinol*** $C_{24}H_{22}O_8$ M 438.433 Isol. from *T. villosa* pods. Mp 200°.

6α,12α-Didehydro: [60077-62-5]. ***Villosol*** $C_{23}H_{20}O_7$ M 408.407 Constit. of the pods of *T. villosa*. Greenish-yellow needles ($CHCl_3$/MeOH). Mp 197°. $[\alpha]_D^{26}$ −80.9° (c, 0.495 in $CHCl_3$).

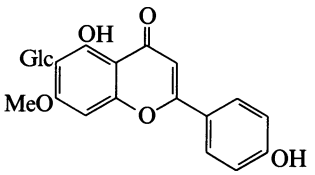
Kerry, T.S. *et al*, *J. Chem. Soc.*, 1939, 1601.
Crombie, L. *et al*, *J. Chem. Soc.*, 1961, 5445.
Crombie, L. *et al*, *J. Chem. Soc.*, 1962, 755 (*pmr*)
Carlson, D.G. *et al*, *Tetrahedron*, 1973, **29**, 2731 (*pmr*)
Crombie, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 1497 (*cmr*)
Sarma, P.N. *et al*, *Indian J. Chem., Sect. B*, 1976, **14**, 152 (*Villosol*)
Krupadanam, G.L.D. *et al*, *Tetrahedron Lett.*, 1977, 2125 (*Villosone, Villinol*)
Uddin, A. *et al*, *Planta Med.*, 1979, **36**, 181; *CA*, **91**, 120359.

Swertisin S-80052

Updated Entry replacing S-01026

6-β-D-Glucopyranosyl-4′,5-dihydroxy-7-methoxyflavone. Flavocommelitin

[6991-10-2]



$C_{22}H_{22}O_{10}$ M 446.410

Constit. of *Swertia japonica* and *S. purpurascens*; *Gaillardia anstata* and *G. pulchella*; *Gentiana campestris* and the aerial parts of *G. germanica*and *G. ramosa*; leaves of *Achillea* genus; of *Dipsacaceae* spp. and petalsof *Iris japonica*. Pale-yellow needles (H_2O). Mp 243° dec. $[\alpha]_D^{20}$ −10.0° (c, 0.9 in Py).

Hexa-Ac: Mp 155-158°.

4′-O-β-D-Glucoside: [16049-42-6]. ***Flavocommelin*** $C_{28}H_{32}O_{15}$ M 608.552 Isol. from *Commelina communis*. Yellow cryst. Mp 216-217°. $[\alpha]_D^{20}$ −40.9° (c, 4.425 in Py).

4′-Me ether: [21089-34-9]. *Embigenin* $C_{23}H_{24}O_{10}$ M 460.437 Mp 236-238°.

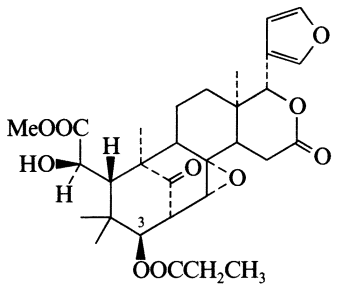
4′-Me ether, 6′-O-α-L-Rhamopyranosyl: [52589-13-6]. ***Embinin*** $C_{29}H_{34}O_{14}$ M 606.579 Isol. from flowers of *I. tectorum* and *I. germaniia*. Mp 180-181°.

Di-Me ether: Mp 302°.

Takeda, K. *et al*, *CA*, 1966, **67**, 99951 (*Flavocommelin*)
Komatsu, M. *et al*, *Tetrahedron Lett.*, 1966, 1611 (*isol*)
Kawase, A. *et al*, *Agric. Biol. Chem.*, 1968, **32**, 537 (*Embigenin*)
Prox, A., *Tetrahedron*, 1968, **24**, 3697 (*ms*)
Wagner, A. *et al*, *Phytochemistry*, 1972, **11**, 851, 1857 (*isol*)
Miana, A.G., *Phytochemistry*, 1973, **12**, 728 (*isol*)
Arisawa, M. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1973, **93**, 1655; *CA*, **80**, 68388q (*Embinin*)
Kaldas, M. *et al*, *Helv. Chim. Acta*, 1975, **58**, 2188 (*isol*)
Zemtsova, G.N. *et al*, *Khim. Prir. Soedin.*, 1977, 705; *CA*, **88**, 60093 (*Glycosides*)

Swietemahonin A S-80053

[121825-44-3]



$C_{30}H_{38}O_{10}$ M 558.624

Constit. of *Swietenia mahogani*. Antagonist of platelet activitating factor. Needles (EtOAc/diisopropyl ether). Mp 174-174.5°. $[\alpha]_D$ −12.2° ($CHCl_3$).

3-O-Deacyl, 3-O-Tigloyl: [121825-42-1]. ***Swietemahonin E***

$C_{32}H_{40}O_{10}$ M 584.662

Constit. of *S. mahogani*. Antagonist of PAF. Needles (EtOAc/diisopropyl ether). Mp 151-152°. $[\alpha]_D$ −20.7° ($CHCl_3$).

Kodota, S. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1111.

Di-Ac:

$C_{31}H_{38}O_{10}$ M 570.635

Constit. of *S. macrophylla*. Cryst. Mp 227-230°. $[\alpha]_D$ −131°.

6-Deoxy: [1915-68-0]. ***6-Deoxyswietenolide***

$C_{27}H_{34}O_7$ M 470.561

Constit. of *Khaya ivorensis*. Cryst. Mp 194-196°. $[\alpha]_D$ −141°.

6-Deoxy, Ac: [1915-69-1]. ***Fissinolide.*** *Grandifoliolin. Augustinolide*

$C_{29}H_{36}O_8$ M 512.599

Constit. of *Cedrela fissilis*, *K. grandifoliola* and *Guarea trichiloides*. Cryst. Mp 169-170°. $[\alpha]_D$ −165°.

6-Deoxy, O-(2-methylpropanoyl): ***Khayasin***

$C_{31}H_{40}O_8$ M 540.652

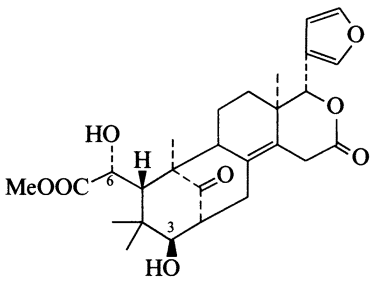
Constit. of *K. senegalensis*. Cryst. (C_6H_6). Mp 114-116°. $[\alpha]_D^{25}$ −165° ($CHCl_3$).

Adesogan, E.K. *et al*, *J. Chem. Soc. C*, 1966, 2127 (*isol, uv, ir, pmr, struct, deriv*)
Chakrabartty, T. *et al*, *Tetrahedron*, 1968, **24**, 1503 (*isol*)
Connolly, J.D. *et al*, *Tetrahedron*, 1968, **24**, 1507 (*struct, pmr*)
Taylor, D.A.H. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 1599; 1974, 437 (*struct, cmr*)
Chan, K.C. *et al*, *Phytochemistry*, 1976, **15**, 429 (*deriv*)
Kadota, S. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1111 (*deriv*)

Swietenolide S-80054

Updated Entry replacing S-01028

[3776-48-5]



$C_{27}H_{34}O_8$ M 486.561

Constit. of the seeds of *Swietenia macrophylla*. Cryst. Mp 221-225°. $[\alpha]_D$ −136° ($CHCl_3$).

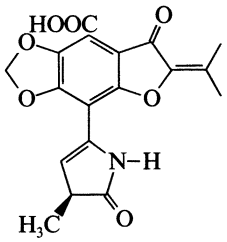
3-Ac: 3-Acetylswietenolide

$C_{29}H_{36}O_9$ M 528.598

Constit. of *S. mahogani*. Needles. Mp 136-138°. $[\alpha]_D$ −17.8° ($CHCl_3$).

Sylvianecic acid S-80055

[80847-64-9]



$C_{18}H_{15}NO_7$ M 357.319

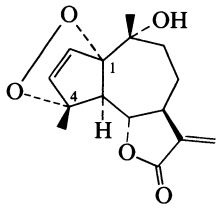
Isol. from an *Aspergillus sylvanecii* strain. Shows antibiotic, antifungal and antitumour activity. Unstable orange cryst. (Me_2CO). Mp 58-59.5°. $[\alpha]_D$ −39.4° ($CHCl_3$).

Yeomans, J.W. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 462 (*isol, cmr, bibl*)

T

Tanaparthin peroxide T-80001

Updated Entry replacing T-20006



$C_{15}H_{18}O_5$ M 278.304

(1α,4α)-form [85799-10-6]

Tanaparthin α-peroxide

Constit. of *Tanacetum parthenium*. Cryst. Mp 95-96°. $[\alpha]_D^{20}$ −32.1° (c, 0.11 in $CHCl_3$).

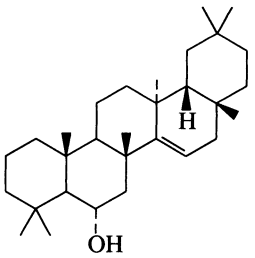
(1β,4β)-form [85758-28-7]

Tanaparthin β-peroxide

Constit. of *T. parthenium*. Gum.

Bohlmann, F. *et al*, *Phytochemistry*, 1982, **21**, 2543 (*isol*)
Begley, M.J. *et al*, *Phytochemistry*, 1989, **28**, 940 (*isol, struct*)

14-Taraxeren-6-ol T-80002



$C_{30}H_{50}O$ M 426.724

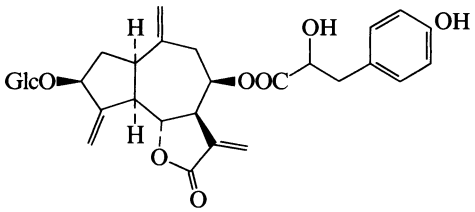
6α-form

Euphorginol

Constit. of *Euphorbia tirucalli*. Cryst. (MeOH). Mp 168-170°. $[\alpha]_D$ +22.35° (c, 0.19 in $CHCl_3$).

Rasool, N. *et al*, *Phytochemistry*, 1989, **28**, 1193.

Tectoroside T-80003



$C_{30}H_{36}O_{12}$ M 588.607

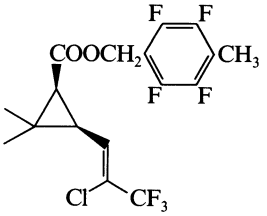
Constit. of *Crepis tectorum*. Oil.

Kisiel, W. *et al*, *Phytochemistry*, 1989, **28**, 2403 (*isol, pmr*)

Tefluthrin T-80004

3-(2-Chloro-3,3,3-trifluro-1-propenyl)-2,2-dimethylcyclopropanecarboxylic acid (2,3,5,6-tetrafluoro-4-methylphenyl)methyl ester, 9CI

[79538-32-2]



$C_{17}H_{14}ClF_7O_2$ M 418.738

Soil-active pyrethroid insecticide. Solid. Mp 44.6°.

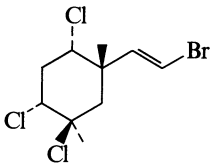
[76437-51-9, 76437-52-0, 79538-33-3]

Japan. Pat., 80 111 445, (1980); *CA*, **94**, 83669q (*synth, use*)
Eur. Pat., 31 199, (1981); *CA*, **95**, 186837t (*synth, use*)

Telfairine T-80005

1-(2-Bromoethenyl)-2,4,5-trichloro-1,5-dimethylcyclohexane

[120163-22-6]



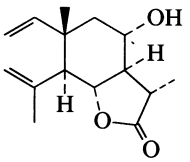
$C_{10}H_{14}BrCl_3$ M 320.483

Constit. of *Plocamium telfairiae*. Amorph. powder (hexane). Mp 62-63°. $[\alpha]_D^{25}$ −18° (c, 0.1 in MeOH).

Watanabe, K. *et al*, *Phytochemistry*, 1989, **28**, 77.

Temisin T-80006

[67151-76-2]



$C_{15}H_{22}O_3$ M 250.337

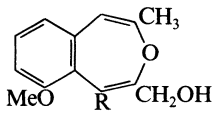
Isol. from *Artemisia maritima*. Prisms (EtOH). Mp 228°. $[\alpha]_D^{20}$ +70° ($CHCl_3$).

(±)-form [67225-38-1]

Mp 196-198°.

Asahina, Y. *et al*, *Ber.*, 1941, **74**, 952 (*isol*)
Nishizawa, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 76 (*struct, synth*)

Tenual T-80007



R = CHO

$C_{14}H_{14}O_4$ M 246.262
Constit. of *Asphodeline tenuior*.

Ulubelen, A. *et al*, *Phytochemistry*, 1989, **28**, 649.

Tenucarb T-80008

As Tenual, T-80007 with

R = COOMe

$C_{15}H_{16}O_5$ M 276.288
Constit. of *Asphodeline tenuior*.

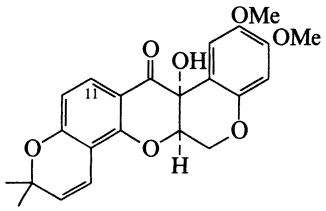
Ulubelen, A. *et al*, *Phytochemistry*, 1989, **28**, 649.

Tephrosin T-80009

Updated Entry replacing T-00140

13,13a-Dihydro-7a-hydroxy-9,10-dimethoxy-3,3-dimethyl-3H-bis[1]benzopyrano[3,4-b:6′,5′-e]pyran-7(7aH)-one, 9CI. Hydroxydeguelin. Allotephrosin. Isoallotephrosin

[76-80-2]



$C_{23}H_{22}O_7$ M 410.423
Found in *Crotalaria burhia*, *C. medicaginea*, *Derris elliptica*, *D. malaccensis*, *Lonchocarpus* spp., *Mundulea sericea*, *Piscidia mollis* and *Tephrosia* spp. Some of these samples are the (−)-form, some the (±)-form and others have unreported opt. activity.

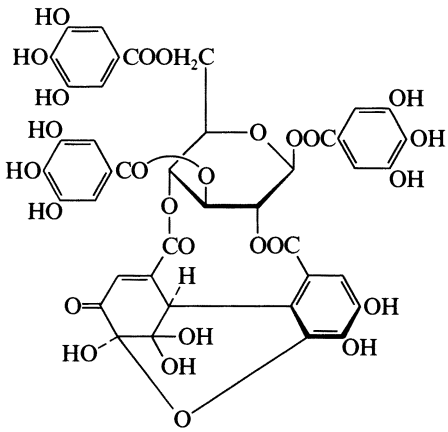
(−)-form
Constit. of the seeds of *Millettia dura*. Amorph. $[\alpha]_D^{23}$ −118° (c, 7.8 in C_6H_6).

11-Hydroxy: [72458-85-6]. ***11-Hydroxytephrosin***
$C_{23}H_{22}O_8$ M 426.422
Isol. from fruit of *A. fruticosa*. Opt. active.

(±)-form
Prisms ($MeOH/CHCl_3$). Mp 198°.

Boam, J.J. *et al*, *J. Soc. Chem. Ind., London*, 1937, **56**, 91 (*rev*)
Ollis, W.D. *et al*, *Tetrahedron*, 1967, **23**, 4741 (*isol, struct*)
Carlson, D.G. *et al*, *Tetrahedron*, 1973, **29**, 2731 (*nmr*)
Braz-Filho, R. *et al*, *Phytochemistry*, 1975, **14**, 1454 (*isol*)
Mitscher, L.A. *et al*, *Heterocycles*, 1979, **12**, 1033 (11-*Hydroxytephrosin*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

Terchebin T-80010



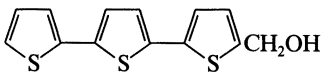
$C_{41}H_{30}O_{26}$ M 938.672
Struct. not certain. Prob. in equilib. with an isomeric struct. Isol. from fruits of *Terminalia chebula*. Small greenish-yellow prisms + $10H_2O$. $[\alpha]_D^{25}$ −39.4° (c, 2 in EtOH). Forms trihydrate on intensive drying.

Schmidt, O.T. *et al*, *Justus Liebigs Ann. Chem.*, 1967, **706**, 169 (*isol*)
Jochims, J.C. *et al*, *Justus Liebigs Ann. Chem.*, 1968, **717**, 769 (*pmr*)
Okuda, T. *et al*, *Tetrahedron Lett.*, 1980, **21**, 4361 (*struct*)
Karl, C. *et al*, *Z. Naturforsch., C*, 1983, **38**, 13 (*struct, pmr*)

2,2′:5′,2″-Terthiophene-5-methanol, 9CI T-80011

5-Hydroxymethyl-2,2′:5,2″-terthiophene. α-Terthienylmethanol

[13059-93-3]



$C_{13}H_{10}OS_3$ M 278.419
Isol. from dried leaves of *Eclipta alba* after hydrol. Lemon-yellow platelets (C_6H_6). Mp 150-151°.

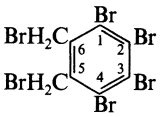
[26905-77-1]

Krishnaswamy, N.R. *et al*, *Curr. Sci.*, 1966, **35**, 542 (*synth*)
Krishnaswamy, N.R. *et al*, *Tetrahedron Lett.*, 1966, 4227 (*isol*)
Nakayama, J. *et al*, *Heterocycles*, 1986, **24**, 637 (*synth*)

1,2,3,4-Tetrabromo-5,6-bis(bromomethyl)benzene, 9CI T-80012

α,α′,3,4,5,6-Hexabromo-o-xylene, 8CI

[53042-28-7]

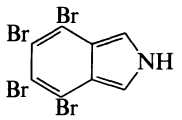


$C_8H_4Br_6$ M 579.544
Cryst. (C_6H_6). Mp 160°.

Hsieh, J.Y.K. *et al*, *Org. Mass Spectrom.*, 1981, **16**, 189 (*ms*)
Kreher, R.P. *et al*, *Chem. Ber.*, 1988, **121**, 1827 (*synth, ir, pmr*)

4,5,6,7-Tetrabromo-2*H*-isoindole T-80013

[52964-20-2]



$C_8H_3Br_4N$ M 432.734
Mp >130° dec.

Kreher, R.P. *et al*, *Chem. Ber.*, 1988, **121**, 1827 (*synth, uv, ir, pmr, cmr, ms*)

Tetrabutylammonium(1+) T-80014

Updated Entry replacing T-30016
N,N,N-*Tributyl-1-butanaminium, 9CI*
[10549-76-5]

$(H_3CCH_2CH_2CH_2)_4N^{\oplus}$

$C_{16}H_{36}N^{\oplus}$ M 242.467 (ion)

Fluoride: [429-41-4].
$C_{16}H_{36}FN$ M 261.465
Catalyst for aldol condensations, acetylations etc. Fluoride ion source. Cryst. + $18H_2O$. Mp 37°. Also forms a hydrate with $32.8H_2O$, Mp 25°.

Azide: [993-22-6].
$C_{16}H_{36}N_4$ M 284.487
Relatively safe azide for synthetic use. Mp 80°.

Borohydride: [33725-74-5].
$C_{16}H_{40}BN$ M 257.310
Reagent for redn. of carboxylic acid to aldehydes. Sol. CH_2Cl_2, insol. Et_2O.

Formate: [35733-58-5].
$C_{17}H_{37}NO_2$ M 287.485
Reagent for OH-group epimerisations.

Iodotetrachloride:
$C_{16}H_{36}Cl_4IN$ M 511.182
Trans-chlorinating agent for alkenes. Mp 137-139° dec.

Chlorochromate: TBACC
$C_{16}H_{36}ClCrNO_3$ M 377.914
Mild, selective oxidising agent. Orange cryst. (EtOAc/hexane). Mp 184-185°.

Hydroxide: [2052-49-5].
$C_{16}H_{37}NO$ M 259.474
Strong base, suitable for use as nonaqueous titrant. Reagent for hydrol. of steroidal tosylates.
▷ BS5425000.

Bifluoride:
$C_{16}H_{37}F_2N$ M 281.472
Fluorinating agent.

Perchlorate: [1923-70-2].
$C_{16}H_{36}ClNO_4$ M 341.917
Needles (EtOAc/pentane). Mp 212.5-213.5°.

Bromide: [1643-19-2].
$C_{16}H_{36}BrNO_4$ M 386.369
Prisms ($CHCl_3$/pet. ether). Mp 119-119.5°.

Tetrafluoroborate: [15553-52-3].
$C_{16}H_{36}BF_4N$ M 329.272
Needles (EtOAc/pentane). Mp 162-162.5°.

Acetate: [10534-59-5].
$C_{18}H_{39}NO_2$ M 301.512
Fine yellow cryst. (1,2-dimethoxyethane). Mp 75-83°. Further purification gave the AcOH solvate, Mp 112.5-114°.

Inorg. Synth., 1957, **5**, 176 (*iodotetrachloride*)
Cundiff, R.H. *et al*, *Anal. Chem.*, 1962, **34**, 584 (*use, hydroxide*)
Gutmann, V. *et al*, *Monatsh. Chem.*, 1964, **95**, 1034 (*azide*)
Wen, W.-Y. *et al*, *J. Phys. Chem.*, 1966, **70**, 1244 (*synth*)
Soriano, J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 209 (*nmr*)
House, H.O. *et al*, *J. Org. Chem.*, 1971, **36**, 2371 (*synth, ir, pmr, bibl*)
Corey, E.J. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 6190 (*synth*)
Brandström, A. *et al*, *Tetrahedron Lett.*, 1972, 3173 (*borohydride*)
Cowell, D.B. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1974, 1505 (*use, hydroxide*)
Pless, J., *J. Org. Chem.*, 1974, **39**, 2644 (*fluoride*)
Kuwajima, J. *et al*, *Synthesis*, 1976, 602 (*fluoride*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 563, 564; 1979, **7**, 353, 354; 1980, **8**, 467; 1981, **9**, 443, 444, 447 (*use*)
Ogilvie, K.K. *et al*, *Tetrahedron Lett.*, 1978, 1663 (*fluoride*)
Sharma, R.K. *et al*, *J. Org. Chem.*, 1983, **48**, 2112 (*props*)
Santaniello, E. *et al*, *Synthesis*, 1983, 749 (*chlorochromate, synth, use*)
Clark, J.H. *et al*, *Tetrahedron Lett.*, 1985, **26**, 2233 (*use, fluoride*)
Bosch, P. *et al*, *Tetrahedron Lett.*, 1987, **28**, 4733 (*bifluoride, synth, use*)

1,1,1,2-Tetrachloro-2-fluoroethane, 9CI T-80015

[354-11-0]

$Cl_3CCHFCl$

C_2HCl_4F M 185.839
d_4^{20} 1.625. Mp −95.4°. Bp 117°. n_D^{20} 1.4525 (1.4488).

Miller, W.T., *J. Am. Chem. Soc.*, 1940, **62**, 341 (*synth*)
Wilmshurst, J.K., *Can. J. Chem.*, 1957, **35**, 937 (*ir*)

1,1,2,2-Tetrachloro-1-fluoroethane, 9CI T-80016

[354-14-3]

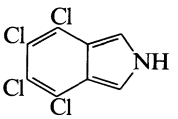
$Cl_2CFCHCl_2$

C_2HCl_4F M 185.839
d_4^{20} 1.622. Bp 115-117°. n_D^{20} 1.4487.

Miller, W.T., *J. Am. Chem. Soc.*, 1940, **62**, 341 (*synth*)
Alger, T.D. *et al*, *J. Chem. Phys.*, 1967, **47**, 3130 (*pmr, F-19 nmr*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1968, **33**, 1294 (*synth*)

4,5,6,7-Tetrachloro-2*H*-isoindole T-80017

[60432-74-8]



$C_8H_3Cl_4N$ M 254.929
Cryst. Mp 200° dec.

Kreher, R.P. *et al*, *Chem. Ber.*, 1988, **121**, 1827 (*synth, uv, ir, pmr, cmr, ms*)

1,1,1,2-Tetrachloro-2,3,3,3-tetrafluoropropane, 9CI, 8CI T-80018

[3175-64-2]

$F_3CCClFCCl_3$

$C_3Cl_4F_4$ M 253.837
d_4^{20} 1.725. Bp 112-112.5°. n_D^{20} 1.4002.

[29255-31-0]

Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 2257 (*synth*)
Paleta, O. *et al*, *Bull. Soc. Chim. Fr.*, 1986, 920 (*synth*)

1,1,1,3-Tetrachloro-2,2,3,3-tetrafluoropropane, 9CI, 8CI — T-80019

[2268-46-4]

$Cl_3CCF_2CClF_2$

$C_3Cl_4F_4$ M 253.837

Solv. for disperse dyes and for glc analysis. Dielectric. Liq. d_4^{25} 1.693. Fp −92.78°. Bp 114°. n_D^{25} 1.3974, n_D^{20} 1.3966.

Coffman, D.D. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 979 (*synth*)
Krespan, C.G. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 3424 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 2257 (*synth*)
Entz, R.C. *et al*, *J. Agric. Food Chem.*, 1982, **30**, 84 (*chromatog*)
Brabets, R. *et al*, *J. Fluorine Chem.*, 1988, **41**, 311 (*props*)

1,1,2,2-Tetrachloro-1,3,3,3-tetrafluoropropane, 8CI — T-80020

[2268-44-2]

$F_3CCCl_2CCl_2F$

$C_3Cl_4F_4$ M 253.837

Hydraulic fluid component. Mp 34°. Bp 112-114°.

[29255-31-0]

McBee, E.T. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 2023 (*synth*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 2257 (*synth*)

1,1,2,3-Tetrachloro-1,2,3,3-tetrafluoropropane, 9CI, 8CI — T-80021

[2268-45-3]

$F_2CClCClFCFCl_2$

$C_3Cl_4F_4$ M 253.837

Liq. (glass at low temp.). d_4^{20} 1.719. Mp −58°. Bp 110-112°. n_D^{20} 1.3960.

[29255-31-0]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 3476 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
Paleta, O. *et al*, *Bull. Soc. Chim. Fr.*, 1986, 920 (*synth*)

1,1,3,3-Tetrachloro-1,2,2,3-tetrafluoropropane, 9CI, 8CI — T-80022

[2354-04-3]

$Cl_2CFCF_2CCl_2F$

$C_3Cl_4F_4$ M 253.837

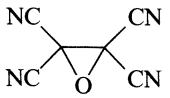
$d^{20}{}_D$ 1.701. Bp 112.5-113.5° (116.5°) . n_D^{20} 1.3980.

Coffman, D.D. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 979 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
White, H.F., *Anal. Chem.*, 1966, **38**, 625 (*F nmr*)

Tetracyanooxirane — T-80023

Oxiranetetracarbonitrile, 9CI. 1,2-Epoxy-1,1,2,2-ethanetetracarbonitrile, 8CI. Tetracyanoethylene oxide

[3189-43-3]



C_6N_4O M 144.092

Needles (1,2-dichloroethane). Mp 177-178° (sealed tube).

▷ Slowly evolves HCN on exposure to H_2O.

Sadtler Standard Infrared Spectra, 23822, 38559P (*ir*)
Reiche, A. *et al*, *Chem. Ber.*, 1963, **96**, 3044 (*synth*)
Linn, W.J. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 2032; 1965, **87**, 3651, 3657, 3665 (*synth*)
Org. Synth., 1969, **49**, 103 (*synth, ir, haz*)
Matthews, D.A. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5945 (*cryst struct*)

Tetracyclo[3.2.0.0^{1,6}.0^{2,6}]heptane, 9CI — T-80024

Tetracyclo[4.1.0.0^{1,5}.0^{2,6}]heptane

[109900-65-4]

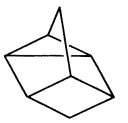
C_7H_8 M 92.140

Bridged [1.1.1]propellane. The higher homologue Tetracyclo[5.1.0.0^{1,6}.0^{2,7}]octane also studied.

Semmler, K. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 6410.
Seiler, P. *et al*, *Helv. Chim. Acta*, 1988, **71**, 2100 (*cryst struct*)

Tetracyclo[3.3.0.0^{2,8}.0^{3,6}]octane, 9CI — T-80025

[5078-81-9]



C_8H_{10} M 106.167

Liq.

Freeman, P.K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1965, 511 (*synth, pmr*)
Freeman, P.K. *et al*, *J. Org. Chem.*, 1973, **38**, 3823 (*synth*)
Bentley, T.W. *et al*, *J. Org. Chem.*, 1988, **53**, 3066 (*synth*)

4,6-Tetradecadiene-8,10-diyne-1,12-diol — T-80026

$H_3CCH_2CH(OH)C{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH_2CH_2CH_2OH$

$C_{14}H_{18}O_2$ M 218.295

(E,E)-form [10523-88-3]

Isol. from above-ground parts of *Cotula coronopifolia*. Cryst. (CCl_4). Mp 55°.

1-Ac: [10523-86-1]. *14-Acetoxy-8,10-tetradecadiene-4,6-diyn-3-ol*

$C_{16}H_{20}O_3$ M 260.332

Isol. from *C. coronopifolia*. Oil. λ_{max} 226, 235.5, 294, 310 nm (Et_2O).

Di-Ac: [20695-84-5]. *1,12-Diacetoxy-4,6-tetradecadiene-8,10-diyne*

$C_{18}H_{22}O_4$ M 302.369

Isol. from *C. coronopifolia*. Oil. λ_{max} 226.5 (ϵ 22800), 236 (34000), 293 (30600), 309 infl. (25400) nm (Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2828; 1968, **100**, 2738 (*isol, uv, ir, pmr, ord, struct, synth*)

6,12-Tetradecadiene-8,10-diyne-1,3-diol — T-80027

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH_2CH_2CH(OH)CH_2CH_2OH$

$C_{14}H_{18}O_2$ M 218.295

(E,E)-form

Pale-yellow amorph. powder. $[\alpha]_D$ +0.73° (c, 1.1 in MeOH).

Di-Ac: [89913-46-2].

$C_{18}H_{22}O_4$ M 302.369

Isol. from Atractylodes Rhizome (*Atractylodes japonica*). Oil. $[\alpha]_D \pm 0°$ (c, 1.7 in MeOH).

Kano, Y. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 193 (*isol, uv, pmr, struct*)

6,12-Tetradecadiene-8,10-diyn-3-ol, 9CI T-80028

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH_2CH_2CH(OH)CH_2CH_3$

$C_{14}H_{18}O$ M 202.296

(E,E)-form

Isol. from roots of *Anthemis suguramica*. Cryst. (pet. ether). Mp 38°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 1642 (*isol, uv, ir, pmr, struct*)

2,12-Tetradecadiene-4,6,8,10-tetrayne T-80029

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH_3$

$C_{14}H_{10}$ M 178.233

Isol. from *Triticum aestivum*. λ_{max} 273 (ϵ 98 400), 292 (75300), 317 (8200), 340 (12100), 365 (13600), 395 nm (7300)(pentane).

Jones, E.R.H. *et al*, *Nature (London)*, 1951, **168**, 900 (*synth, uv*)
Schulte, H.E. *et al*, *Phytochemistry*, 1965, **4**, 481 (*isol, uv*)

5,7,9,11-Tetradecatetraen-1-ol T-80030

$H_3CCH_2(CH{=}CH)_4CH_2CH_2CH_2CH_2OH$

$C_{14}H_{22}O$ M 206.327

(5E,7E,9Z,11E)-form

Centaur Y

Isol. from above-ground parts of *Centaurea cyanus* and *C. ruthenica*. Cryst. (pet. ether). Mp 48-50°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1961, **94**, 3179; 1962, **95**, 2939 (*isol, uv, ir, struct, synth*)

4,6,10,12-Tetradecatetraen-8-yn-1-ol, 9CI T-80031

[16692-74-3]

$H_3CCH{=}CHCH{=}CHC{\equiv}CCH{=}CHCH{=}CHCH_2CH_2CH_2OH$

$C_{14}H_{18}O$ M 202.296

(all-E)-form [10523-90-7]

Isol. from roots of *Saussurea alpina* and from *Zoegea baldschuanica*. Cryst. (pet. ether). Mp 94-95°.

Ac: [13028-52-9]. *14-Acetoxy-2,4,8,10-tetradecaen-6-yne*
$C_{16}H_{20}O_2$ M 244.333
Isol. from above-ground parts of *Cotula coronopifolia*. Cryst. (pet. ether). Mp 32°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 2828, 3201 (*isol, uv, ir, pmr, struct*)

4,6,12-Tetradecatrien-8,10-diyn-1-ol, 9CI T-80032

[13081-23-7]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH_2CH_2CH_2OH$

$C_{14}H_{16}O$ M 200.280

(E,E,E)-form [17090-99-2]

Isol. from *Dahlia merckii* and roots of *Anthemis saguramica*. Platelets (Et_2O/pet. ether). Mp 110-111°.

Ac: [1540-89-2].
$C_{16}H_{18}O_2$ M 242.317

Isol. from *A. carpatica*, *D. merckii*, *Cotula coronopifolia* and other plants. Cryst. (pet. ether). Mp 31-33°.

Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1963, **668**, 51 (*isol, deriv*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 872; 1966, **99**, 1642, 3544 (*isol uv, ir, pmr, struct, synth*)
Sörensen, J.S. *et al*, *Acta Chem. Scand.*, 1966, **20**, 992 (*isol, synth*)
Aplin, R.T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 140 (*ms*)
Bedford, C.T., *J. Chem. Soc., Perkin Trans.* 1, 1976, 735 (*isol, synth*)

4,6,12-Tetradecatriene-8,10-diyne-1,3-diol T-80033

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHC{=}CHCH(OH)CH_2CH_2OH$

$C_{14}H_{16}O_2$ M 216.279

(all-E)-form

Di-Ac:
$C_{18}H_{20}O_4$ M 300.354
Isol. from *Atraclylodes japonica*. Pale-yellow oil. $[\alpha]_D$ +0.4° (c, 1.0 in MeOH).

Kano, Y. *et al*, *Chem. Pharm. Bull.*, 1989, **37**, 193 (*isol, ir, uv, pmr, ms*)

2-Tetradecene, 9CI, 8CI T-80034

[1652-97-7]

$H_3C(CH_2)_{10}CH{=}CHCH_3$

$C_{14}H_{28}$ M 196.375

(E)-form [35953-54-9]

Liq. Bp 253°.

(Z)-form [35953-53-8]

Liq. Bp 253.9°.

Janak, J., *Anal. Chem.*, 1973, **45**, 293 (*chromatog*)
Uemura, S. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 2748 (*synth*)
Polyakova, A.A. *et al*, *Zh. Org. Khim.*, 1987, **23**, 1164 (*ms*)

3-Tetradecene, 9CI, 8CI T-80035

[36587-78-7]

$H_3C(CH_2)_9CH{=}CHCH_2CH_3$

$C_{14}H_{28}$ M 196.375

(E)-form

Liq. Bp 251.4°.

(Z)-form

Liq. Bp 251.3°.

Janak, J., *Anal. Chem.*, 1973, **45**, 293 (*chromatog*)
Polyakova, A.A. *et al*, *Zh. Org. Khim.*, 1987, **23**, 1164 (*ms*)

4-Tetradecene, 9CI, 8CI T-80036

[54322-28-0]

$H_3C(CH_2)_8CH{=}CHCH_2CH_2CH_3$

$C_{14}H_{28}$ M 196.375

(E)-form [41446-78-0]

Liq. Bp 250.9°.

(Z)-form [41446-65-5]

Liq. Bp 250.5°.

Janak, J., *Anal. Chem.*, 1973, **45**, 293 (*chromatog*)
Polyakova, A.A., *Zh. Org. Khim.*, 1987, **23**, 1164 (*ms*)

5-Tetradecene, 9CI, 8CI T-80037

$H_3C(CH_2)_7CH{=}CH(CH_2)_3CH_3$

$C_{14}H_{28}$ M 196.375

(*E*)-*form* [41446-66-6]
Liq. Bp 250.8°, $Bp_{0.1}$ 56-61°. n_D^{20} 1.4365.

(*Z*)-*form* [41446-62-2]
Bp 250°.

Janak, J., *Anal. Chem.*, 1973, **45**, 293 (*chromatog*)
Batchelor, J.G. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6358 (*cmr*)
Commercon, A. *et al*, *Tetrahedron Lett.*, 1975, 3837 (*synth*)
Neumann, H. *et al*, *Chem. Ber.*, 1978, **111**, 2785 (*synth, ir, pmr*)
Brown, H.C. *et al*, *J. Org. Chem.*, 1986, **26**, 5270 (*synth*)
Polyakova, A.A. *et al*, *Zh. Org. Khim.*, 1987, **23**, 1164 (*ms*)

6-Tetradecene, 9CI, 8CI T-80038

[23015-35-2]

$H_3C(CH_2)_6CH{=}CH(CH_2)_4CH_3$

$C_{14}H_{28}$ M 196.375

(*E*)-*form* [41446-64-4]
Liq. Bp 250.4°.

(*Z*)-*form* [41446-61-1]
Liq. Bp 249.6°.

Meshcheryakov, A.P. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1958, 780; *ca*, **52**, 19974 (*synth*)
Janak, J., *Anal. Chem.*, 1973, **45**, 293 (*chromatog*)
Polyakova, A.A. *et al*, *Zh. Org. Khim.*, 1987, **23**, 1164 (*ms*)

7-Tetradecene, 9CI, 8CI T-80039

[10374-74-0]

$H_3C(CH_2)_5CH{=}CH(CH_2)_5CH_3$

$C_{14}H_{28}$ M 196.375

(*E*)-*form* [41446-63-3]
Liq. Bp 250.2°.

(*Z*)-*form* [41446-60-0]
Liq. Bp 249.4°, $Bp_{0.8}$ 75-76°. n_D^{20} 1.4399.

Sadtler Standard Infrared Spectra, 40362 (*ir*)
Sadtler Standard NMR Spectra, 9909 (*pmr*)
Janak, J., *Anal. Chem.*, 1973, **45**, 293 (*chromatog*)
Brown, H.C. *et al*, *J. Org. Chem.*, 1982, **47**, 3806, 3808; 1986, **26**, 5270; 1988, **53**, 239 (*synth, pmr*)
Julia, M. *et al*, *Tetrahedron Lett.*, 1982, **23**, 2457 (*synth*)
Polyakova, A.A. *et al*, *Zh. Org. Khim.*, 1987, **23**, 1164 (*ms*)

8-Tetradecene-11,13-diyn-2-one, 9CI T-80040

[115006-46-7]

$HC{\equiv}CC{\equiv}CCH_2CH{=}CH(CH_2)_5COCH_3$

$C_{14}H_{18}O$ M 202.296

(*Z*)-*form* [13945-78-3]
Isol. from roots of *Centaurea pullata* and *C. ferox*. Present in *Echinacea* spp. Oil.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 3544 (*isol, ir, pmr, ms, struct*)
Heinzer, F. *et al*, *Pharm. Acta Helv.*, 1988, **63**, 132; *ca*, **109**, 146331z (*isol*)

9-Tetradecene-2,4,6-triynedioic acid, 9CI T-80041

$HOOC(CH_2)_3CH{=}CHCH_2C{\equiv}CC{\equiv}CC{\equiv}CCOOH$

$C_{14}H_{12}O_4$ M 244.246

(*Z*)-*form* [109921-61-1]
Isol. from *Poria sinuosa*. Amorph. unstable solid. Dec. at ca. 120°.

Cambie, R.C. *et al*, *J. Chem. Soc.*, 1963, 2065 (*isol, uv, ir, struct*)

5-Tetradecene-8,10,12-triyn-1-ol T-80042

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH_2CH{=}CH(CH_2)_3CH_2OH$

$C_{14}H_{16}O$ M 200.280

(*Z*)-*form*
Ac: 13-Acetoxy-9-tetradecene-2,4,6-triyne
$C_{16}H_{18}O_2$ M 242.317
Isol. from above-ground parts of *Chrysanthemum serotinum*. Oil.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 1830 (*isol, ir, uv, pmr, struct*)

6-Tetradecene-8,10,12-triyn-3-ol T-80043

$H_3C(C{\equiv}C)_3CH{=}CHCH_2CH_2CH(OH)CH_2CH_3$

$C_{14}H_{16}O$ M 200.280

(−)-(*E*)-*form*
Isol. from *Anacyclus pyrethrum* and *Anthemis saguramica*. Cryst. (pet. ether). $[\alpha]_D^{22}$ −56° (c, 0.25 in Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1411; 1966, **99**, 1642 (*isol, uv, ir, pmr, ord, struct*)

3-Tetradecenoic acid T-80044

$H_3C(CH_2)_9CH{=}CHCH_2COOH$

$C_{14}H_{26}O_2$ M 226.358

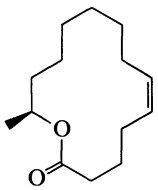
(*E*)-*form* [75730-21-1]
Isol. from seed oil of *Grindelia oxylepis*.

[62472-83-7, 81236-42-2]

Kleiman, R. *et al*, *Lipids*, 1966, **1**, 301 (*isol*)
Gunstone, F.D. *et al*, *Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Mizugaki, M. *et al*, *Chem. Pharm. Bull.*, 1980, **28**, 2347 (*nmr*)
Ogura, K. *et al*, *Tetrahedron Lett.*, 1981, **22**, 4499 (*synth*)

5-Tetradecen-13-olide T-80045

14-Methyloxacyclotetradec-6-en-2-one, 9CI



$C_{14}H_{24}O_2$ M 224.342

(*S,Z*)-*form* [87420-69-7]
Synergist of aggregation pheromone of *Cryptolestes puscillus*. Oil. $[\alpha]_D^{23}$ +54.4° (c, 1.275 in $CHCl_3$).

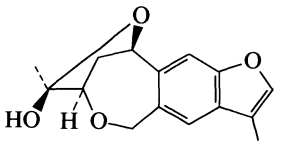
[77761-59-2, 78418-66-3, 87420-70-0]

Millar, J.G. *et al*, *J. Org. Chem.*, 1983, **48**, 4404 (*synth*)
Millar, J.G. *et al*, *J. Chem. Ecol.*, 1985, **11**, 1053 (*synth*)
Sakai, T. *et al*, *Agric. Biol. Chem.*, 1986, **50**, 1621 (*synth*)
Naoshima, Y. *et al*, *Chem. Lett.*, 1989, 1023 (*synth, isol*)

5,6,9,10-Tetradehydro-1,4:3,14-diepoxy-4-hydroxy-4,5-secofuranoeremophilane **T-80046**

5,7,8,10-Tetrahydro-3,8-dimethyl-7,10-methanofuro[2,3-i][2,5]benzodioxocin-8-ol, 9CI

[53820-32-9]



$C_{15}H_{16}O_4$ M 260.289

Constit. of *Euryops hebecarpus*. Oil. λ_{max} 250, 275, 281 nm.

Bohlmann, F. *et al*, *Chem. Ber.*, 1974, **107**, 2730.

Tetraethoxyethene, 9CI **T-80047**

Tetraethoxyethylene

[40923-93-1]

$(EtO)_2C{=}C(OEt)_2$

$C_{10}H_{20}O_4$ M 204.266

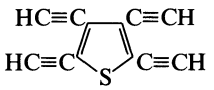
Bp_{15} 77°. n_D^{25} 1.4212.

McElvain, S.M. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 2661 (*synth*)

Scheeren, J.W. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1973, **92**, 11 (*synth*)

Tetraethynylthiophene **T-80048**

[113705-25-2]



$C_{12}H_4S$ M 180.230

Solid. Unstable, rapidly turns black on standing in air.

▷ Explosive. Heat and shock sensitive, exploded on attempted subl.

Neenan, T.X. *et al*, *J. Org. Chem.*, 1988, **53**, 2489 (*synth, pmr, cmr, ms, uv, haz*)

Tetrafluorobutanedioic acid, 9CI **T-80049**

Updated Entry replacing T-00642

Tetrafluorosuccinic acid. Perfluorosuccinic acid

[377-38-8]

$HOOCCF_2CF_2COOH$

$C_4H_2F_4O_4$ M 190.051

Mp 116°. Bp_{15} 150°.

▷ WN0725000.

Hydrate: Mp 86.4-87.4°.

Dianilinium salt: Cryst. ($EtOH/CHCl_3$). Mp 224°.

Di-Me ester: [356-36-5].

$C_6H_6F_4O_4$ M 218.105

Bp 177-178°.

Di-Et ester:

$C_8H_{10}F_4O_4$ M 246.158

Liq. d_4^{20} 1.26. Bp_{15} 89°.

Dichloride: [356-15-0].

$C_4Cl_2F_4O_2$ M 226.942

Bp 86.1-86.3°.

Diamide:

$C_4H_4F_4N_2O_2$ M 188.081

Cryst. (H_2O). Mp 261°.

Dianilide: Cryst. (Me_2CO aq.). Mp 227.5-228°.

Anhydride: [699-30-9]. *3,3,4,4-Tetrafluorodihydro-2,5-furandione, 9CI. Tetrafluorosuccinic anhydride*

$C_4F_4O_3$ M 172.036

Cryst. d_4^{20} 1.61. Mp 54-56°.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 281 (*synth*)

Haszeldine, R.N., *J. Chem. Soc.*, 1954, 4026 (*synth*)

Fear, E.J.P. *et al*, *J. Appl. Chem.*, 1955, **5**, 589 (*ester, anhydride, synth*)

Fear, E.J.P. *et al*, *J. Chem. Soc.*, 1956, 3199 (*synth, anhydride, chloride, amide*)

1,1,2,2-Tetrafluoro-1,2-diiodoethane, 9CI **T-80050**

1,2-Diiodoperfluoroethane. sym-*Diiodotetrafluoroethane*

[354-65-4]

F_2ClCF_2I

$C_2F_4I_2$ M 353.825

d_4^{25} 2.629. Bp 112-113°, Bp_{14} 23°. n_D^{25} 1.489.

Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co., 079 (*F*-19 *nmr*)

Emeleus, H.J. *et al*, *J. Chem. Soc.*, 1949, 2948 (*synth*)

Coffman, D.D. *et al*, *J. Org. Chem.*, 1949, **14**, 747 (*synth*)

Nodiff, E.A. *et al*, *J. Org. Chem.*, 1953, **18**, 235 (*props*)

Knunyants, I.L. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1964, 384 (*synth*)

Chung Wu, E. *et al*, *J. Phys. Chem.*, 1975, **79**, 1078 (*uv*)

Powell, D.L. *et al*, *J. Raman Spectrosc.*, 1978, **7**, 111 (*ir, raman*)

Ulm, K. *et al*, *Toxicol. Lett.*, 1980, **6**, 365 (*tox*)

1,1,2,2-Tetrafluoroethane, 9CI **T-80051**

[430-66-0]

F_2CHCHF_2

$C_2H_2F_4$ M 102.031

Gas. Bp −22.5°.

▷ Flammable.

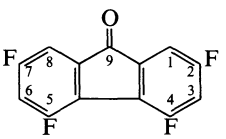
Young, D.S. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 1171 (*synth*)

Knunyants, I.L. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1958, 906 (*synth*)

Dean, R.R. *et al*, *Trans. Faraday Soc.*, 1968, **64**, 1409 (*pmr, F*-19 *nmr*)

2,4,5,7-Tetrafluoro-9*H*-fluoren-9-one **T-80052**

[114995-45-8]

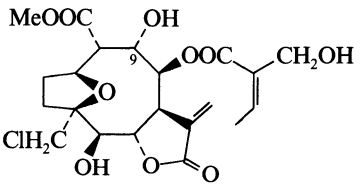


$C_{13}H_4F_4O$ M 252.168

Bright yellow cryst. solid (EtOAc/hexane). $Bp_{0.25}$ 70° subl.

Kyba, E. *et al*, *J. Org. Chem.*, 1988, **53**, 3513 (*synth, cmr*)

Tetragonolide **T-80053**



$C_{21}H_{27}ClO_{10}$ M 474.891

9-(2-Methylpropanoyl): [119886-36-1]. *Tetragonolide isobutyrate*

$C_{25}H_{33}ClO_{11}$ M 544.982

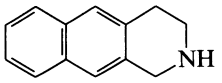
Constit. of *Tetragonotheca repanda* and *T. ludoviciana*. Oil.

9-(2-Methylbutanoyl): [119863-95-5]. *Tetragonolide 2-methylbutyrate*
$C_{26}H_{35}ClO_{11}$ M 559.009
Constit. of *T. ludoviciana*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 3881.

1,2,3,4-Tetrahydrobenz[g]isoquinoline T-80054

[21628-46-6]



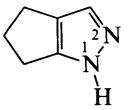
$C_{13}H_{13}N$ M 183.252
Cryst. (pet. ether). Mp 121°.

B,HCl: [112576-43-9].
Cryst. Mp 290-295°.

N-*Ac:*
$C_{15}H_{15}NO$ M 225.290
Cryst. (cyclohexane). Mp 157°.

Etienne, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **267**, 1826 (*synth*)
Young, S.D. *et al*, *J. Org. Chem.*, 1988, **53**, 1114 (*synth, pmr*)

1,4,5,6-Tetrahydrocyclopentapyrazole, 9CI T-80055



$C_6H_8N_2$ M 108.143

1H-form [2214-03-1]
Cryst. (MeOH). Mp 57-59°. Bp_{30} 165°.

2H-form [15409-55-9]
Derivs. have various commercial uses.

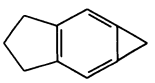
2-Ph: [120344-42-5].
$C_{12}H_{12}N_2$ M 184.240
Cryst. Mp 79°.

2-Benzyl: [84597-88-6].
$C_{13}H_{14}N_2$ M 198.267
Liq. $Bp_{2.5}$ 160°.

Wallach, O., *Justus Liebigs Ann. Chem.*, 1903, **329**, 109 (*synth*)
Bardou, L. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 289 (*synth*)
Gustafsson, H. *et al*, *Acta Chem. Scand.*, *Ser. B*, 1974, **28**, 1069 (*synth, pmr*)
Aubert, T. *et al*, *Synthesis*, 1988, 742 (*synth, ir, pmr, ms, use, bibl*)

1,3,4,5-Tetrahydrocycloprop[f]indene T-80056

[112504-81-1]



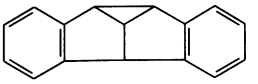
$C_{10}H_{10}$ M 130.189
Pale yellow oil.

Billups, W.E. *et al*, *J. Org. Chem.*, 1988, **53**, 1312 (*synth, ir, pmr*)

4*b*,8*b*,8*c*,8*d*-Tetrahydrodibenzo[*a*,*f*]cyclopropa[*cd*]pentalene T-80057

Dibenzotricyclo[3.3.0.0^{2,8}]octa-3,6-diene. Dibenzosemibullvalene

[2199-28-2]



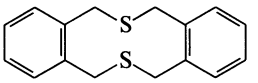
$C_{16}H_{12}$ M 204.271
Cryst. (Pet. ether). Mp 104-105°.

Ciganek, E., *J. Am. Chem. Soc.*, 1966, **88**, 2882 (*synth*)
Cristol, S.J. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 401 (*synth*)

5,7,12,14-Tetrahydrodibenzo[*c*,*h*][1,6]dithiecin, 9CI T-80058

2,11-Dithia[3.3]orthocyclophane

[7215-69-2]



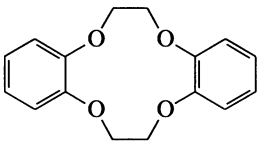
$C_{16}H_{16}S_2$ M 272.434
Needles (C_6H_6). Mp 249-251° (244-246°).

Au, M.-K. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1979, 1475 (*synth, pmr*)
Lai, Y.-H. *et al*, *J. Org. Chem.*, 1988, **53**, 2360 (*synth, pmr, ir, uv, ms, conformn*)

6,7,14,15-Tetrahydrodibenzo[*b*,*h*][1,4,7,10]tetraoxacyclododecin, 9CI T-80059

Dibenzo-12-crown-4

[14696-05-0]

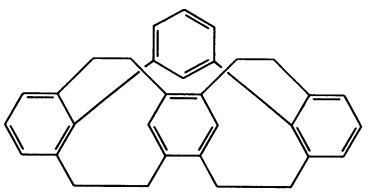


$C_{16}H_{16}O_4$ M 272.300
Mp 208-209°.

Pedersen, C.J., *J. Am. Chem. Soc.*, 1967, **89**, 7017 (*synth*)
Charland, J.P. *et al*, *Acta Crystallogr.*, *Sect. C*, 1989, **45**, 165 (*cryst struct*)

5,6,20,21-Tetrahydro-2,16;3,10-diethano-15,11-metheno-11*H*-tribenzo[*a*,*e*,*i*]pentadecene, 9CI T-80060

[116129-69-2]

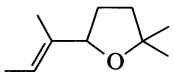


$C_{32}H_{28}$ M 412.573
Mp 266°.

Vinod, T.K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6574 (*synth*)

Tetrahydro-2,2-dimethyl-5-(1-methyl-1-propenyl)furan **T-80061**

[7416-35-5]



$C_{10}H_{18}O$ M 154.252

Isol. from oil of *Citrus aurantifolia*. Oil. d^{20} 0.867. $[\alpha]_D^{20}$ $\pm 0°$. n_D^{20} 1.4662.

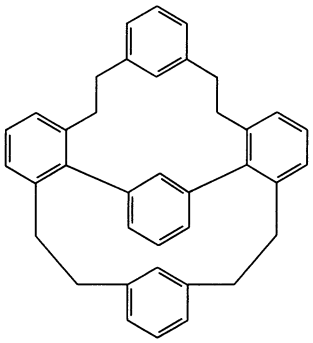
[56058-69-6, 56058-70-9]

Kováts, E. *et al*, *Helv. Chim. Acta*, 1963, **46**, 2705; 1966, **49**, 2055 (*isol*)

Corbier, B. *et al*, *Recherches*, 1974, **19**, 235 (*synth*)

5,6,12,13-Tetrahydro-1,17-(ethano[1,3]benzenoethano)-7,11:18,22-dimethenodibenzo[*a*,*h*]cyclooctadecene, 9CI **T-80062**

[116129-64-7]



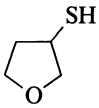
$C_{38}H_{34}$ M 490.687

Cup-shaped molecule. Mp 210°. *o* and *p* -analogues also prepd.

Vinod, T.K. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6574 (*synth*)

Tetrahydro-3-furanthiol **T-80063**

3-Mercaptotetrahydrofuran



C_4H_8OS M 104.173

(±)-***form***

Ph thioether: [64823-94-5]. *Tetrahydro-3-(phenythio)furan, 9CI*

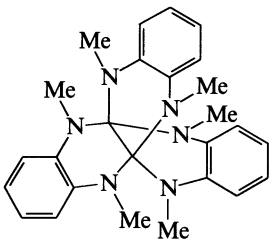
$C_{10}H_{12}OS$ M 180.270

Oil.

Abd El Samii, Z.K.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 2509 (*synth, ir, pmr, cmr*)

5,6,11,12-Tetrahydro-5,6,11,12,13,20-hexamethyl-5*a*,11*a*-(imino[1,2]benzenimino)quinoxalino[2,3-*b*]quinoxaline, 9CI **T-80064**

[118894-97-6]



$C_{26}H_{30}N_6$ M 426.563

Cryst. (EtOH). Mp 272-273°.

Tauer, E. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 338 (*synth, uv, pmr*)

1,2,3,4-Tetrahydro-5-hydroxyisoquinoline **T-80065**

1,2,3,4-Tetrahydro-5-quinolinol. 5-Hydroxy-1,2,3,4-tetrahydroisoquinoline

[102877-50-9]

$C_9H_{11}NO$ M 149.192

Cryst. (MeOH or by subl.). Mp 273°.

B,HCl: [102879-34-5].

Cryst. (EtOH/Et_2O). Mp 257.6-259.7°.

Me ether; BHCl: [103030-69-9].

$C_{10}H_{13}NO$ M 163.219

Cryst. (EtOH/Et_2O). Mp 234.9-236.0°.

[103030-70-2]

Durand, S. *et al*, *Bull. Soc. Chim. Fr.*, 1961, 270 (*synth, deriv*)

Schenker, F. *et al*, *J. Heterocycl. Chem.*, 1971, **8**, 665 (*synth, pmr*)

Sall, D.J. *et al*, *J. Med. Chem.*, 1987, **30**, 2208 (*synth, deriv, pmr, ir, cmr, ms*)

1,2,3,4-Tetrahydro-7-hydroxyisoquinoline **T-80066**

Updated Entry replacing H-03450

1,2,3,4-Tetrahydro-7-isoquinolinol, 9CI. 7-Hydroxy-1,2,3,4-tetrahydroisoquinoline

[30798-64-2]

$C_9H_{11}NO$ M 149.192

Bp_{18} 210-220°.

B,HBr: [110192-19-3].

Cryst. (EtOH). Mp 210.3-211.4°.

Me ether: [43207-78-9]. ***Weberidine.*** *1,2,3,4-Tetrahydro-7-methoxyisoquinoline, 9CI*

$C_{10}H_{13}NO$ M 163.219

Alkaloid from *Pachycereus weberi* (Cactaceae). $Bp_{0.1}$ 115° (synth.) .

Me ether; B,HCl: Mp 233° (228°).

Pictet, A. *et al*, *Ber.*, 1911, **44**, 2036 (*synth*)

Schenker, F. *et al*, *J. Heterocycl. Chem.*, 1971, **8**, 665 (*synth, pmr*)

Moniot, J.L. *et al*, *Heterocycles*, 1978, **9**, 145 (*pmr*)

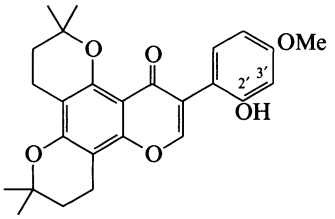
Mata, R. *et al*, *Phytochemistry*, 1980, **19**, 673 (*isol, uv, ir, pmr, ms, synth, deriv*)

Mata, R. *et al*, *Phytochemistry*, 1983, **22**, 1263 (*cmr, deriv*)

Sall, D.J. *et al*, *J. Med. Chem.*, 1987, **30**, 2208 (*synth, pmr, ir, cmr, ms*)

3,4,7,8-Tetrahydro-11-(2-hydroxy-4-methoxyphenyl)-2,2,6,6-tetramethyl-2*H*,6*H*,12*H*-benzo[1,2-*b*;3,4-*b*′;5,6-*b*″]tripyran-12-one, 9CI T-80067

[78876-34-3]



$C_{26}H_{28}O_6$ M 436.504
Isol. from leaves of *Millettia pachycarpa*. Cryst. (EtOAc/pet. ether). Mp 165°.

2′-Deoxy, 3′-hydroxy:
$C_{26}H_{28}O_6$ M 436.504
Isol. from leaves of *M. pachycarpa*. Noncryst. Struct. not certain. May have the alternative 4′-hydroxy-3′-methoxy struct. (preferred on balance).

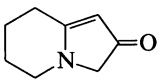
[78876-33-2]

Singhal, A.K. *et al*, *Phytochemistry*, 1981, **20**, 803.

5,6,7,8-Tetrahydro-2(3*H*)-indolizinone, 9CI T-80068

2,3,5,6,7,8-Tetrahydroindolizin-2-one

[97202-63-6]

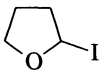


$C_8H_{11}NO$ M 137.181
Oil. $Bp_{0.0002}$ 69°.

Pommelet, J.C. *et al*, *J. Org. Chem.*, 1988, **53**, 5680 (*synth, ir, pmr, cmr, ms*)

Tetrahydro-2-iodofuran T-80069

3-Iodooxolane



C_4H_7IO M 198.003

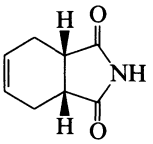
(±)-*form*
$Bp_{0.2}$ 40°.

Evans, R.D. *et al*, *Synthesis*, 1988, 862 (*synth, pmr, ir*)

3*a*,4,7,7*a*-Tetrahydro-1*H*-isoindole-1,3(2*H*)-dione, 9CI T-80070

1,2,3,6-Tetrahydrophthalimide. 4-Cyclohexene-1,2-dicarboximide

[85-40-5]



$C_8H_9NO_2$ M 151.165

(*3aRS,7aSR*)-*form* [1469-48-3]
cis-*form*
Cryst. (EtOH). Mp 136-138°.

▷ Toxic.

Ag salt: [62506-08-5].
Tan powder.

N-*Me:* [62950-21-4].
$C_9H_{11}NO_2$ M 165.191
Cryst. (C_6H_6/hexane). Mp 72.5-73° (60-62°).

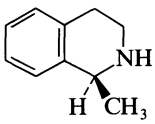
[2015-58-9, 5167-69-1]

Rice, L.M. *et al*, *J. Org. Chem.*, 1954, 884 (*synth, deriv*)
Christol, H. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 1315 (*synth*)
Kirfel, A., *Acta Crystallogr.*, 1976, 1556 (*cryst struct*)
Evans, D.L. *et al*, *J. Org. Chem.*, 1979, **44**, 497 (*deriv, pmr*)
Crockett, G.C. *et al*, *Synth. Commun.*, 1981, 447 (*synth*)
Wijnberg, B.P. *et al*, *Tetrahedron*, 1982, **38**, 209 (*synth*)
Caswell, L.R. *et al*, *J. Org. Chem.*, 1984, **49**, 696 (*synth*)
Mori, M. *et al*, *Tetrahedron Lett.*, 1987, 6187.

1,2,3,4-Tetrahydro-1-methylisoquinoline T-80071

Updated Entry replacing T-00917

[4965-09-7]



(*S*)-*form*

$C_{10}H_{13}N$ M 147.219

(*S*)-*form*
Oil. $[\alpha]_D^{25}$ −71.3° (c, 0.64 in THF).

B,HCl: Cryst. Mp 208°.

(±)-*form*
Oil. Bp_{745} 233°.

B,HCl: Mp 173°.

Picrate: Mp 187°.

[64982-61-2, 64982-62-3]

Robinson, R. *et al*, *J. Org. Chem.*, 1951, **16**, 1911 (*synth*)
Sakane, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1974, **45**, 1297 (*use*)
Meyers, A.I. *et al*, *Tetrahedron*, 1987, **43**, 5095 (*synth, pmr, ir*)

Tetrahydro-3-methyl-2*H*-pyran T-80072

3-Methyltetrahydropyran

[26093-63-0]

$C_6H_{12}O$ M 100.160
d_4^{20} 0.863. Bp 109°.

(±)-*form*
d_4^{20} 0.86. Bp_{733} 109°.

Hanschke, E., *Chem. Ber.*, 1955, **88**, 1048.

Tetrahydro-4-methyl-2*H*-pyran, 9CI T-80073

4-Methyltetrahydropyran

[4717-96-8]

$C_6H_{12}O$ M 100.160

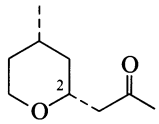
(±)-*form*
Liq.

Booth, H. *et al*, *Tetrahedron*, 1987, **43**, 4699 (*synth, pmr, cmr, conformn*)

(Tetrahydro-4-methyl-2*H*-pyran-2-yl)-2-propanone, 9CI **T-80074**

2-Acetonyl-4-methyltetrahydropyran. Rose oxide ketone

[20194-70-1]



$C_9H_{16}O_2$ M 156.224

Used in perfumery.

(2R*,4S*)-form [73127-43-2]

cis-*form*

Isol. from geranium oil (*Pelargonium roseum*). d_4^{20} 0.956. Bp_{14} 87-88°. $[\alpha]_D$ −1.5°. n_D^{20} 1.4460.

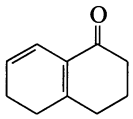
Naves, Y.R. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1608 (*isol, ir, pmr, synth*)

Japan. Pat., 74 85 071, (1974); *CA*, **82**, 31256k (*synth*)

Japan. Pat., 74 85 072, (1974); *CA*, **82**, 31255j (*synth*)

3,4,5,6-Tetrahydro-1(2*H*)-naphthalenone **T-80075**

[113668-50-1]



$C_{10}H_{12}O$ M 148.204

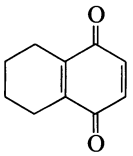
Oil. Unstable, gradually aromatises.

Marcinow, Z. *et al*, *J. Org. Chem.*, 1988, **53**, 2117 (*synth, ir, pmr*)

5,6,7,8-Tetrahydro-1,4-naphthoquinone, 8CI **T-80076**

5,6,7,8-Tetrahydro-1,4-naphthalenedione, 9CI

[7474-90-0]



$C_{10}H_{10}O_2$ M 162.188

Yellow needles (pet.ether). Mp 55-56°.

Monoxime: [22658-31-7].

$C_{10}H_{11}NO_2$ M 177.202

Cryst. (xylene). Mp 167-168°.

Arnold, R.T. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 1317 (*synth*)

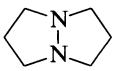
Fr. Pat., 1 508 481, (1968); *CA*, **71**, 3132w (*oxime*)

Malesani, G. *et al*, *J. Heterocycl. Chem.*, 1982, **19**, 633 (*ir, pmr*)

Tetrahydro-1*H*,5*H*-pyrazolo[1,2-*a*]pyrazole, 9CI **T-80077**

*1,5-Diazabicyclo[3.3.0]octane. Octahydro-3*a*,6*a*-diazapentalene. 8-Azapyrrolizidine. 1,2-Trimethylenepyrazolidine. Perhydro-3*a*,6*a*-diazapentalene*

[5397-67-1]



$C_6H_{12}N_2$ M 112.174

Oil, freezing to plates. d_{20}^{20} 1.00. Mp 1.5-2.5°. Bp 173°, Bp_{26} 74-75°. n_D^{20} 1.4895.

Picrate: Mp 159.5°.

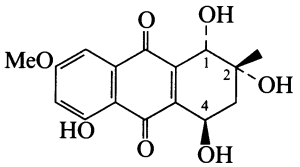
Buhle, E.L. *et al*, *J. Am. Chem. Soc.*, 1943, **65**, 29 (*synth*)

Stetter, H. *et al*, *Chem. Ber.*, 1965, **98**, 3228 (*synth*)

Koopmann, H.P. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 157 (*ir, raman*)

Nelsen, S.F. *et al*, *J. Org. Chem.*, 1980, **45**, 3609 (*nmr*)

1,2,3,4-Tetrahydro-1,2,4,5-tetrahydroxy-7-methoxy-2-methylanthraquinone **T-80078**



(1*S*,2*R*,4*R*)-*form*

$C_{16}H_{16}O_7$ M 320.298

(1S,2R,4R)-form

Constit. of fungus *Dermocybe* sp. Yellow cryst. Mp 72-75°. $[\alpha]_D$ −323° (c, 0.35 in $CHCl_3$).

(1S,2R,4S)-form

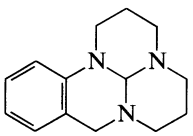
Constit. of *D.* sp. Yellow cryst. Mp 74-80°. $[\alpha]_{365}$ +350° (c, 0.6 in $CHCl_3$).

(1S,2S,4R)-form

Constit. of *D.* sp. Yellow cryst. Mp 93-98°. $[\alpha]_D$ −152° ($CHCl_3$).

Burns, C.J. *et al*, *Tetrahedron Lett.*, 1989, **30**, 7269 (*isol, synth*)

2,3,5,6-Tetrahydro-1*H*,4*H*,7*H*,11*cH*-3*a*,6*a*,11*b*-triazabenz[*de*]anthracene, 9CI **T-80079**



$C_{14}H_{19}N_3$ M 229.324

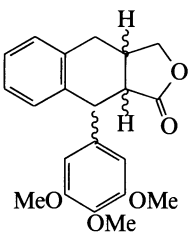
(±)-*form* [112672-92-1]

Cryst. Mp 78-80°.

Beddoes, R.L. *et al*, *Tetrahedron*, 1987, **43**, 1903 (*synth, uv, ir, pmr, ms, cryst struct*)

3*a*,4,9,9*a*-Tetrahydro-9-(3,4,5-trimethoxyphenyl)naphtho[2,3-*c*]furan-1(3*H*)one **T-80080**

1,2,3,4-Tetrahydro-3-(hydroxymethyl)-1-(3,4,5-trimethoxyphenyl)-2-naphthalenecarboxylic acid lactone

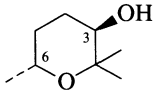


$C_{21}H_{22}O_5$ M 354.402

Isol. from seed oil of *Hernandia ovigera*. Lignan of deoxypodophyllotoxin type.

Hata, C., *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1942, **63**, 1540; *CA*, **41**, 2917.

Tetrahydro-2,2,6-trimethyl-2*H*-pyran-3-ol, 9CI T-80081



(3*R*,6*R*)-*form*

$C_8H_{16}O_2$ M 144.213

Volatile component from the elm bark beetle *Pteleobius vittatus*. Stereochem. of nat. prod. not yet known.

(3R,6R)-form [111465-16-8]
(+)-*trans-form*
Needles (hexane). Mp 37.3-38.5°. $[\alpha]_D^{25}$ +12.6° (c, 0.99 in Et_2O).

(3R,6S)-form [111465-17-9]
(−)-cis-*form*
Needles (hexane). Mp 47.5-48.5°. $[\alpha]_D^{24}$ −31.7° (c, 0.50 in Et_2O).

(3S,6R)-form [111465-15-7]
(+)-cis-*form*
Needles (hexane). Mp 48-48.5°. $[\alpha]_D^{25}$ +32.6° (c, 0.84 in Et_2O).

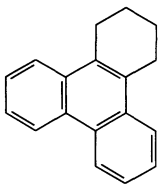
(3S,6S)-form [111465-18-0]
(−)-trans-*form*
Needles (hexane). Mp 37.5-38°. $[\alpha]_D^{24}$ −11.8° (c, 0.95 in Et_2O).

[93172-43-1, 107536-57-2]

Mori, K. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 175 (*synth, ir, pmr, cmr, ms, ord*)

1,2,3,4-Tetrahydrotriphenylene, 9CI T-80082

9,10-Cyclohexenophenanthrene



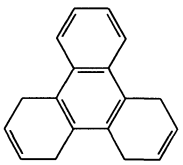
$C_{18}H_{16}$ M 232.324

Needles (1-propanol). Mp 120-121°.

Bergmann, E. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 1441 (*synth*)
Fu, P.P. *et al*, *J. Org. Chem.*, 1980, **45**, 2797 (*synth, pmr*)
Penn, J.H. *et al*, *J. Org. Chem.*, 1989, **54**, 601 (*synth, uv, ir, pmr, cmr, ms*)

1,4,5,8-Tetrahydrotriphenylene T-80083

[114249-91-1]

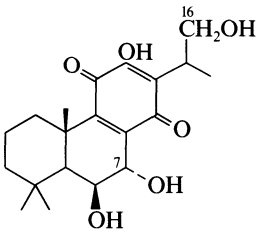


$C_{18}H_{16}$ M 232.324

Cryst. (EtOH). Mp 199-200°.

Marcinow, Z. *et al*, *J. Org. Chem.*, 1988, **53**, 3603 (*synth, pmr*)

6,7,12,16-Tetrahydroxy-8,12-abietadiene-11,14-dione T-80084



$C_{20}H_{28}O_6$ M 364.438

(6β,7α)-form

7-Ac: [120462-43-3]. ***Lophanthoidin C***
$C_{22}H_{30}O_7$ M 406.475
Constit. of *R. lophanthoides*. Cryst. Mp 167-169.5°.

16-Ac: [120462-45-5]. ***Lophanthoidin E***
$C_{22}H_{30}O_7$ M 406.475
Constit. of *R. lophanthoides*. Cryst. Mp 152.5-154°.

7,16-Di-Ac: [120462-42-2]. ***Lophanthoidin B***
$C_{24}H_{32}O_8$ M 448.512
Constit. of *R. lophanthoides*. Cryst. Mp 138-139°.

7-Me ether, 16-Ac: [120462-41-1]. ***Lophanthoidin A***
$C_{23}H_{32}O_7$ M 420.502
Constit. of *Rabdosia lophanthoides*. Cryst. Mp 198-202°.

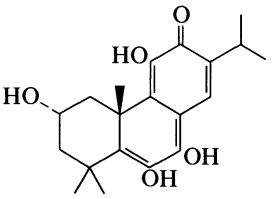
7-Et ether: [120462-44-4]. ***Lophanthoidin D***
$C_{22}H_{32}O_6$ M 392.491
Constit. of *R. lophanthoides*. Cryst. Mp 205-210°.

7-Et ether, 16-Ac: [120462-46-6]. ***Lophanthoidin F***
$C_{24}H_{34}O_7$ M 434.528
Constit. of *R. lophanthoides*. Cryst. Mp 184-185°.

Yunlong, X. *et al*, *Phytochemistry*, 1989, **28**, 189.

2,6,7,11-Tetrahydroxy-5,7,9(11),13-abietatetraen-12-one T-80085

5,6-Didehydro-2,7-dihydroxytaxodone



$C_{20}H_{26}O_5$ M 346.422

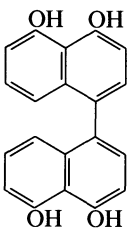
2α-form

Constit. of *Salvia texana*. Cryst. ($CHCl_3$).

Gonzalez, A.G. *et al*, *Tetrahedron*, 1989, **45**, 5203.

4,4′,5,5′-Tetrahydroxy-1,1′-binaphthyl T-80086

[*1,1′-Binaphthalene*]-*4,4′,5,5′-tetrol*



$C_{20}H_{14}O_4$ M 318.328

Metab. of *Daldinia concentrica*. Pale-yellow cryst.

Tetra-Ac:

$C_{28}H_{22}O_8$ M 486.477
Mp 245°.

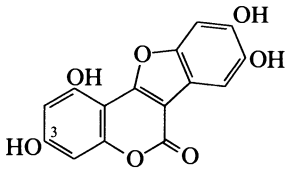
Allport, D.C. *et al*, *J. Chem. Soc.*, 1958, 4090; 1960, 654.

1,3,8,9-Tetrahydroxycoumestan T-80087

Updated Entry replacing W-00012

1,3,8,9-Tetrahydroxy-6H-benzofuro[3,2-c][1]benzopyran-6-one, 9CI, 8CI. 5,7,11,12-Tetrahydroxycoumestan. ***Desmethylwedelolactone.*** *Norwedelolactone. Demethylwedelolactone*

[6468-55-9]



$C_{15}H_8O_7$ M 300.224
Constit. of *Wedelia calendulacea* and *Eclipta alba*. Mp >360°.

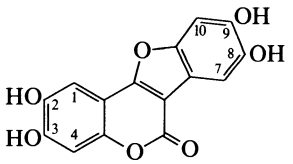
3-O-Glucoside: [30414-09-6].
$C_{21}H_{18}O_{12}$ M 462.366
Isol. from leaves of *E. alba*. Mp >340°.

Tetra-Ac: Mp 270-272°.

O³-Me: [524-12-9]. *5,11,12-trihydroxy-7-methoxycoumestan.* ***Wedelolactone***
$C_{16}H_{10}O_7$ M 314.251
Constit. of *W. calendulacea* and *E. alba*. Greenish-yellow needles (MeOH). Mp 327-330° dec.

Govidachari, T.R. *et al*, *J. Chem. Soc.*, 1956, 629; 1957, 545, 548 (*isol, struct, ir, Wedelolactone*)
Khastgir, H.N. *et al*, *Tetrahedron*, 1961, **14**, 257 (*uv*)
Wanzlick, H.W. *et al*, *Chem. Ber.*, 1963, **96**, 305 (*synth*)
Chatterjea, J.N. *et al*, *Chem. Ber.*, 1964, **97**, 1252 (*synth*)
Bhargava, K.K. *et al*, *Indian J. Chem.*, 1970, **8**, 664; 1972, **10**, 810 (*isol, struct*)

2,3,8,9-Tetrahydroxycoumestan T-80088



$C_{15}H_8O_7$ M 300.224

2-Me, 8,9-methylene ether: [75656-29-0]. *3-Hydroxy-2-methoxy-8,9-methylenedioxycoumestan.* ***Tephrosol***
$C_{17}H_{10}O_7$ M 326.262
Constit. of *Tephrosia villosa* root. Yellow-green cryst. (MeOH). Mp 306°.

3-Me, 8,9-methylene ether: [35930-39-3]. ***2-Hydroxy-3-methoxy-8,9-methylenedioxycoumestan.*** *2-Hydroxyflemichapparin C*
$C_{17}H_{10}O_7$ M 326.262
Isol. from heartwood of *Swartzia leiocalycina*.

Donnelly, D.M.X. *et al*, *Phytochemistry*, 1971, **10**, 3147 (*isol*)
Rao, D.D. *et al*, *Phytochemistry*, 1980, **19**, 1272 (*isol*)

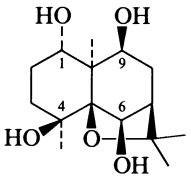
3,4,8,9-Tetrahydroxycoumestan T-80089

$C_{15}H_8O_7$ M 300.224

4-Me,8,9-methylene ether: [79295-80-0]. *3-Hydroxy-4-methoxy-8,9-methylenedioxycoumestan.* ***Sophoracoumestan*** **B**
$C_{17}H_{10}O_7$ M 326.262
Isol. from roots of *Sophora franchetiana*. Needles (MeOH). Mp >300°.

Komatsu, M. *et al*, *Chem. Pharm. Bull.*, 1981, **29**, 2069 (*isol, uv, pmr, struct*)

1,4,6,9-Tetrahydroxydihydro-β-agarofuran T-80090



$C_{15}H_{26}O_5$ M 286.367

(1α,4β,6β,9β)-form

9-Ac,1-benzoyl: 9β-Acetoxy-1α-benzoyloxy-4β,6β-dihydroxydihydro-β-agarofuran
$C_{24}H_{32}O_7$ M 432.513
Constit. of *Orthosphenia mexicana*.

6,9-Di-Ac,1-benzoyl: 6β,9β-Diacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran
$C_{26}H_{34}O_8$ M 474.550
Constit. of *O. mexicana*. Cryst. Mp 202°.

González, A.G. *et al*, *Phytochemistry*, 1988, **27**, 473.

2′,5,6′,7-Tetrahydroxyflavone T-80091

Updated Entry replacing T-50153

2-(2,6-Dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. ***Argemexitin***

[82475-00-1]

$C_{15}H_{10}O_6$ M 286.240
Constit. of *Argemone mexicana*. Yellow needles (EtOH). Mp >330°.

2′-Me ether: [92519-94-3]. *2′,5,7-Trihydroxy-6′-methoxyflavone*
$C_{16}H_{12}O_6$ M 300.267
Isol. from root of *Scutellaria baicalensis*. Cryst. (MeOH). Mp 256-257° dec.

Bhardwaj, D.K. *et al*, *Phytochemistry*, 1982, **21**, 2154 (*isol*)
Tomimuri, T. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1984, **104**, 529 (*ir, isol, uv, pmr, cmr, ms*)
Tanaka, T. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1987, **107**, 315 (*synth*)

3′,4′,6,7-Tetrahydroxyflavone T-80092

Updated Entry replacing T-30091

$C_{15}H_{10}O_6$ M 286.240
Yellow cryst. Mp >320°.

3,6-Di-Me ether: [68007-24-9]. *4′,7-Dihydroxy-3,6-dimethoxyflavone*
$C_{17}H_{14}O_6$ M 314.294
Isol. from *Pluchea chingoyo*.

4′,6-Di-Me ether: 3′,7-Dihydroxy-4′,6-dimethoxyflavone. ***Abrectorin***
$C_{17}H_{14}O_6$ M 314.294
Constit. of *Abrus precatorius*. Cryst. (EtOH). Mp 229-230°, Mp 273-274°.

6,7-Di-Me ether: [123442-39-7]. *3,4′-Dihydroxy-6,7-dimethoxyflavone.* ***Hortensin***
$C_{17}H_{14}O_6$ M 314.294
Constit. of *Millingtonia hortensis*. Pale yellow cryst. Mp 212-213°.

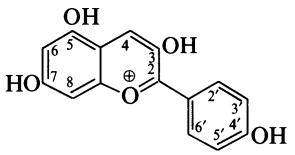
Tetra-Me ether: 3′,4′,6,7-Tetramethoxyflavone

$C_{19}H_{18}O_6$ M 342.348
Needles ($CHCl_3$/pet. ether). Mp 221-222°.

Chiang, M.T. *et al*, *Rev. Latinoam. Quim.*, 1978, **9**, 102 (*isol*)
Bhardwaj, D.K. *et al*, *Phytochemistry*, 1980, **19**, 2040 (*isol, struct, ir, uv*)
Bhardwaj, D.K. *et al*, *Indian J. Chem., Sect. B*, 1982, **21**, 98 (*synth*)
Bunyapraphatsara, N. *et al*, *Phytochemistry*, 1989, **28**, 1555 (*Hortensin*)

3,4′,5,7-Tetrahydroxyflavylium, 8CI T-80093

Updated Entry replacing T-01248
3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-1-benzopyrylium, 9CI. ***Pelargonidin***
[7690-51-9]



$C_{15}H_{11}O_5^{\oplus}$ M 271.249
Anthocyanin pigment present in many plants, flowers and fruits, e.g. radishes, orchids, brassicas, *Petunia* spp. Glycosides also widely distributed. Ms unsuitable as analytical technique.

Chloride: [134-04-3].
$C_{15}H_{11}ClO_5$ M 306.702
Leaflets (MeOH/Et_2O), needles (MeOH/HCl). Mod. sol. H_2O. Mp >350°.

3-β-D-Glucoside: [18466-51-8]. ***Callistephin***
$C_{21}H_{21}O_{10}^{\oplus}$ M 433.391
Pigment from scarlet carnations. Red cryst. (as chloride).

5-β-D-Glucoside: ***Pelargonenin***
$C_{21}H_{21}O_{10}^{\oplus}$ M 433.391
Scarlet-red needles (as chloride). Spar. sol. H_2O. Red col. with bluish fluor. in acid soln., viol.-blue col. in aq. Na_2CO_3 soln.

7-Glucoside:
$C_{21}H_{21}O_{10}^{\oplus}$ M 433.391
Scarlet needles (as chloride). Na_2CO_3 aq. → deep pink col.

4′-Glucoside:
$C_{21}H_{21}O_{10}^{\oplus}$ M 433.391
Red plates (as chloride). Dec. at 184°.

3,5-Diglucoside: [17334-58-6]. ***Pelargonin.*** *Monardin. Salvinin*
$C_{27}H_{31}O_{15}^{\oplus}$ M 595.533
Fine red needles + $4H_2O$ (as chloride). Sol. H_2O. Mp 180° dec. (anhyd.) (chloride). $[\alpha]_D$ −244°. Orange-red soln. in H_2O turning viol. on standing. MeOH soln. red with green fluor.

3-Galactoside: ***Fragarin***
$C_{21}H_{21}O_{10}^{\oplus}$ M 433.391
Isol. from leaves of *Fagus sylvatica* var. *purpurea* as chloride. λ_{max} 278, 505 nm (MeOH/HCl).

3-O-[2-O-β-D-Xylopyranosyl(1→2)-α-D-glucopyranoside]: Pelargonidin 3-sambubioside
$C_{26}H_{29}O_{14}^{\oplus}$ M 565.507
Isol. from petals of *Streptocarpus* spp. (as chloride) and present in other members of the Gesneriaceae. λ_{max} 277, 508 nm (MeOH/HCl).

3-O-[β-D-Glucopyranosyl(1→2)-β-D-glucopyranoside]: Pelargonidin 3-sophoroside
$C_{27}H_{31}O_{15}^{\oplus}$ M 595.533
Isol. from petals of *Papaver rhoeas* and *P. orientale* (as chloride). λ_{max} 268, 505 nm (MeOH/HCl).

3-O-[β-D-Glucopyranosyl(1→2$_{glu}$)[α-L-rhamnopyranosyl(1→6)-β-D-glucopyranoside]]: Pelargonidin 3-(2^{glu}glucosylrutinoside)
$C_{33}H_{41}O_{19}$ M 741.675
Isol. from fruits of *Rubus idaeus* (as chloride). λ_{max} 275, 508 nm (MeOH/HCl).

3-O-[β-D-Xylopyranosyl(1→2)-β-D-glucopyranoside], 5-O-β-D-glucopyranoside: Pelagonidin 5-glucoside 3-sambubioside
$C_{32}H_{39}O_{19}^{\oplus}$ M 727.649
Isol. from petals of *Matthiola incana* (as chloride). λ_{max} 280, 508 nm (MeOH/HCl). Present in acylated form in the plant.

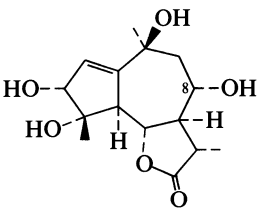
3-O-[β-D-Glucopyranosyl(1→2)-β-D-glucopyranoside], 5-O-β-D-glucopyranoside: Pelargonidin 5-glucoside 3-sophoroside
$C_{33}H_{41}O_{20}$ M 757.675
Present in acylated form in roots of *Raphanus sativus*.

3-O-Sophoroside, 7-O-glucoside: ***Orientalin†***
$C_{33}H_{41}O_{20}^{\oplus}$ M 757.675
Isol. from petals of *Papaver* and *Watsonia* spp. (as chloride). λ_{max} 279, 499 nm (MeOH/HCl). Orientaline is also the name of an alkaloid.

3-O-[α-L-Rhamnopyranosyl(1→6)-β-D-glucopyranoside], 5-O-glucoside: Pelargonidin 5-glucoside 3-rutinoside
$C_{33}H_{41}O_{19}^{\oplus}$ M 741.675
Present in petals of *Dichrotrichum* sp. and in *Achimenes* spp.

Robertson, A. *et al*, *J. Chem. Soc.*, 1928, 1460, 1533 (*isol*)
Léon, A. *et al*, *J. Chem. Soc.*, 1931, 2673 (*synth, glucosides*)
Harborne, J.B. *et al*, *Phytochemistry*, 1963, **2**, 85; 1964, **3**, 453; 1966, **5**, 589 (*isol*)
Timberlake, C.F. *et al*, *Nature (London)*, 1966, **212**, 158 (*uv*)
Nilson, E., *Chem. Scr.*, 1973, **4**, 49 (*pmr*)
Timberlake, C.F. *et al*, *The Flavonoids*, (Harbourne, J.B. etal, Eds.), Chapman and Hall, 1975, 215 (*rev*)
Saito, N. *et al*, *Heterocycles*, 1985, **23**, 2709 (*cryst struct*)

3,4,8,10-Tetrahydroxy-1-guaien-12,6-olide T-80094



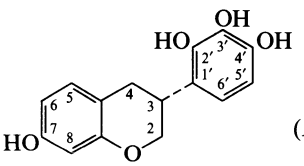
$C_{15}H_{22}O_6$ M 298.335
(3α,4α,5α,6α,7α,8α,10β,11S)-form

8-Ac: [119403-32-6]. *8α-Acetoxy-3α,4α,10β-trihydroxy-1-guaien-12,6α-olide*
$C_{17}H_{24}O_7$ M 340.372
Constit. of *Artemisia arborescens*. Cryst. (EtOH). Mp 140-145°.

Grandolini, G. *et al*, *Phytochemistry*, 1988, **27**, 3670 (*isol, pmr*)

2′,3′,4′,7-Tetrahydroxyisoflavan T-80095

3,4-Dihydro-7-hydroxy-3-(2,3,4-trihydroxyphenyl)-2H-1-benzopyran



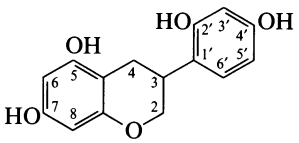
(R)-form

$C_{15}H_{14}O_5$ M 274.273

3′,4′-Di-Me ether: [64474-51-7]. *2′,7-Dihydroxy-3′,4′-dimethoxyisoflavan.* ***Isomucronulatol***
$C_{17}H_{18}O_5$ M 302.326
Isol. from *Astragalus glycyphyllos, A. penduliflorus, Carmichaelia flagelliformis, Colutea arborescens, Gliricidia sepium* and *Glycyrrhiza glabra*. Cryst. (MeOH aq.). Mp 152-153°. $[\alpha]_D^{20}$ −19.4° (c, 0.24 in EtOH).

Al-Ani, H.A.M. *et al, Phytochemistry*, 1985, **24**, 55 (*biosynth, bibl, Isomucronulatol*)

2′,4′,5,7-Tetrahydroxyisoflavan T-80096



$C_{15}H_{14}O_5$ M 274.273
No obt. rotns. or chiralities reported for nat. prods.

4′,5-Di-Me ether: [73354-16-2]. *2′,7-Dihydroxy-4′,5-dimethoxyisoflavan. 5-Methoxyvestitol*
$C_{17}H_{18}O_5$ M 302.326
Stress metab. from *Lotus edulis* and *L. hispidus*.

5,7-Di-Me ether: [77370-02-6]. *2′,4′-Dihydroxy-5,7-dimethoxyisoflavan.* ***Lotisoflavan***
$C_{17}H_{18}O_5$ M 302.326
Stress metab. from leaves of *L. angustissimus* and *L. edulis*. Mp 135-137° (synth. racemate).

Ingham, J.L. *et al, Phytochemistry*, 1979, **18**, 1711; 1980, **19**, 2799 (*isol, uv, ms, struct*)

2′,4′,5′,7-Tetrahydroxyisoflavan T-80097

3,4-Dihydro-7-hydroxy-3-(2,4,5-trihydroxyphenyl)-2H-1-benzopyran

$C_{15}H_{14}O_5$ M 274.273

4′,5′-Methylene ether: [57436-37-0]. *2′,7-Dihydroxy-4′,5′-methylenedioxyisoflavan.* ***Maackiainisoflavan.*** *Dihydromaackiain*
$C_{16}H_{14}O_5$ M 286.284
Isol. from cultures of *Stemphylum botryosum* as metab. of Maackiain.

2′-Me, 4′,5′-methylene ether: [72026-91-6]. *7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavan.* ***Astraciceran***
$C_{17}H_{16}O_5$ M 300.310
Isol. from leaves of *Astragalus cicer* and *A. pyrenaicus*. Phytoalexin. Cryst. (MeOH). Mp 168°.

[22091-12-9]

Higgins, V.J., *Physiol. Plant Pathol.*, 1975, **6**, 5 (*Maackianisoflavan*)
Ingham, J.L. *et al, Phytochemistry*, 1980, **19**, 1767 (*Astraciceran*)

2′,4′,6,7-Tetrahydroxyisoflavan T-80098

3,4-Dihydro-3-(2,4-dihydroxyphenyl)-6,7-dihydroxy-2H-1-benzopyran

$C_{15}H_{14}O_5$ M 274.273

4′,6-Di-Me ether: [56752-02-4]. *2′,7-Dihydroxy-4′,6-dimethoxyisoflavan. 6-Methoxyvestitol*
$C_{17}H_{18}O_5$ M 302.326
Isol. from cultures of *Fusarium solani* growing on *Pisum sativum*.

Pueppke, S.G. *et al, Physiol. Plant Pathol.*, 1976, **8**, 51.

2′,3′,4′,7-Tetrahydroxyisoflavanone T-80099

2,3-Dihydro-7-hydroxy-3-(2,3,4-trihydroxyphenyl)-4H-1-benzopyran-4-one

$C_{15}H_{12}O_6$ M 288.256

(±)-form

2′,3′-Di-Me ether: [79852-12-3]. *4′,7-Dihydroxy-2′,3′-dimethoxyisoflavanone.* ***Lespedeol C***
$C_{17}H_{16}O_6$ M 316.310
Isol. from heartwood of *Lespedeza cyrtobotrya*. Needles (Me_2CO/hexane). Mp 206-209°.

2′,4′-Di-Me ether: [52250-38-1]. *3′,7-Dihydroxy-2′,4′-dimethoxyisoflavanone.* ***Violanone***
$C_{17}H_{16}O_6$ M 316.310
Isol. from heartwoods of *Dalbergia violacea* and *D. oliveri*. Mp 200-202°.

2′,3′,4′-Tri-Me ether: [56973-42-3]. *7-Hydroxy-2′,3′,4′-trimethoxyisoflavanone. 3′-O-Methylviolanone*
$C_{18}H_{18}O_6$ M 330.337
Isol. from wood of *D. cearensis*. Cryst. (C_6H_6/MeOH). Mp 192-194°.

3′,4′,7-Tri-Me ether: [71973-13-2]. *2′-Hydroxy-3′,4′,7-trimethoxyisoflavanone. 3′-Methoxyisosativanone*
$C_{18}H_{18}O_6$ M 330.337
Isol. from trunkwood of *Myroxylon peruiferum*. Mp 155-157°. Racemic.

Donnelly, D.M.X. *et al, Phytochemistry*, 1974, **13**, 2587 (*Violanone*)
Guimarães, I.S. . de S. *et al, Phytochemistry*, 1975, **14**, 1452 (3′-*O*-Methylviolanone)
Maranduba, A. *et al, Phytochemistry*, 1979, **18**, 815 (3′-*Methoxyisosativanone*)
Miyase, T. *et al, Chem. Pharm. Bull.*, 1981, **29**, 2205 (*Lespedeol C*)

2′,4′,5,7-Tetrahydroxyisoflavanone T-80100

Updated Entry replacing T-03370

2,3-Dihydro-5,7-dihydroxy-3-(2,4-dihydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Dalbergioidin***

[30368-42-4]

$C_{15}H_{12}O_6$ M 288.256
Isol. from *Dolichos biflorus, Lablab niger, Lespedeza cyrtobotrya, Macrotyloma axillare, Ougeinia dalbergiodes, Phaseolus vulgaris* and *Stizolobium deeringianum* (all Leguminosae, Papilionoideae).

2′-Me ether: [76656-75-2]. *4′,5,7-Trihydroxy-2′-methoxyisoflavanone.* ***Isoferreirin***
$C_{16}H_{14}O_6$ M 302.283
Constit. of *D. biflorus* and *S. deeringianum*.

4′-Me ether: [32898-79-6]. *2′,5,7-Trihydroxy-4′-methoxyisoflavanone.* ***Ferreirin***
Isol. from heartwood of *Ferreirea spectabilis* also from *Haplormosia monophylla* and *Cajanus cajan*. Prisms (MeOH aq. or pet. ether). Mp 210-212°.

2′,4-Di-Me ether: [482-01-9]. *5,7-Dihydroxy-2′,4′-dimethoxyisoflavanone.* ***Homoferreirin***
$C_{17}H_{16}O_6$ M 316.310
Isol. from *Argyrocytisus battandieri, Cicer arietinum, Ferreirea spectabilis* and *O.dalbergioides*. Rectangular plates (C_6H_6/pet. ether or MeOH aq.). Mp 168-169°.

2′,4′-Di-Me ether,di-Ac: Long needles. Mp 132-133°.

2′,7-Di-Me ether: [61020-70-0]. *4′,5-Dihydroxy-2′,7-dimethoxyflavanone.* ***Cajanol***
$C_{17}H_{16}O_6$ M 316.310

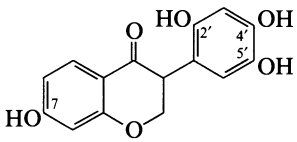
Isol. from fungus-infected stems of *Cajanus cajan* and *S. deeringainum*. Revised struct. Formerly considered to be 2′,6-Dihydroxy-4′,7-dimethoxyisoflavanone.

Tetra-Me ether: [28812-39-7]. *2′,4′,5,7-Tetramethoxyisoflavanone*
$C_{19}H_{20}O_6$ M 344.363
Cryst. (C_6H_6). Mp 163°.

King, F.E. *et al*, *J. Chem. Soc.*, 1952, 4580, 4752 (*Ferreirin, Homoferreirin*)
Farkas, L. *et al*, *J. Chem. Soc. C*, 1971, 1994 (*synth*)
Ingham, J.L. *et al*, *Z. Naturforsch.*, *C*, 1976, **31**, 504; 1977, **32**, 1018; 1980, **35**, 923 (*isol, spectra, biosynth, derivs*)
Woodward, M.D., *Phytochemistry*, 1979, **18**, 363 (*isol*)
Ingham, J.L., *Z. Naturforsch.*, *C*, 1979, **34**, 159 (*Cajanol*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

2′,4′,5′,7-Tetrahydroxyisoflavanone T-80101

Updated Entry replacing H-20201



$C_{15}H_{12}O_6$ M 288.256

4′,5′-Methylene ether: [524-08-3]. *2′,7-Dihydroxy-4′,5′-methylenedioxyisoflavanone.* ***Sophorol***
$C_{16}H_{12}O_6$ M 300.267
Isol. from heartwood of *Sophora japonica*. Plates (Me_2CO aq.). Mp 180-181° (after drying). $[\alpha]_D^{15}$ +9.5° (Me_2CO), $[\alpha]_D^{16}$ −13.6° (EtOH).

2′-Me, 4′,5′-methylene ether: [58116-57-7]. *7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavanone.* ***Onogenin***
$C_{17}H_{14}O_6$ M 314.294
Isol. from *Dalbergia stevensonii* and *Ononis arvensis*. Prisms (pet. ether). Mp 213-214° (189-193°). Racemic.

(±)-***form*** [51106-85-5]
Constit. of *Dalbergia stevensonii* and *Ononis arvensis*. Prisms (C_6H_6/pet. ether). Mp 189-193°, Mp 213-214°.

Suginome, H., *J. Org. Chem.*, 1959, **24**, 1655 (*Sophorol*)
Donnelly, D.M.X. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1973, 1737 (*isol*)
Farkas, L. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1974, 305 (*synth*)
Kovalev, V.N. *et al*, *Khim. Prir. Soedin.*, 1975, **11**, 354 (*isol*)

3′,4′,6,7-Tetrahydroxyisoflavanone T-80102

Updated Entry replacing D-05381

$C_{15}H_{10}O_6$ M 286.240

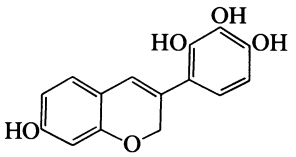
6,7-Di-Me, 3′,4′-methylene ether: [24195-20-8]. *6,7-Dimethoxy-3′,4′-methylenedioxyisoflavanone*
$C_{18}H_{16}O_6$ M 328.321
Constit. of the heartwoods of *Cordyla africana* and *Mildbraedeodendron excelsa*. Needles ($CHCl_3$/MeOH). Mp 201.5-202.5°.

Campbell, R.V.M. *et al*, *J. Chem. Soc. C*, 1969, 1787 (*isol, struct, synth*)
Aggarwal, S.K. *et al*, *Indian J. Chem.*, 1972, **10**, 804 (*synth*)
Meegan, M.J. *et al*, *Phytochemistry*, 1975, **14**, 2283 (*isol*)

2′,3′,4′,7-Tetrahydroxyisoflavene T-80103

Updated Entry replacing S-00299

4-(7-Hydroxy-2H-1-benzopyran-3-yl)-6-methoxy-1,2,3-benzenetriol, 9CI



$C_{15}H_{12}O_5$ M 272.257

3′-Me ether: [79852-14-5]. *2′,4,7-Trihydroxy-3′-methoxyisoflavene.* ***Haginin C***
$C_{16}H_{14}O_5$ M 286.284
Isol. from heartwood of *Lespedeza cyrtobotrya*.

3′-Me ether, tri-Ac: Needles (CH_2Cl_2/MeOH). Mp 138-139.5°.

4′-Me ether: [60434-16-4]. *2′,3′,7-Trihydroxy-4′-methoxyisoflavene.* ***Sepiol***
$C_{16}H_{14}O_5$ M 286.284
Constit. of *Gliricidia sepium* heartwood. Brownish prisms (MeOH aq.). Mp 209-210°.

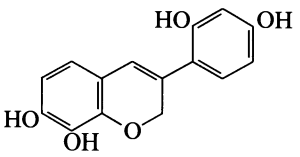
2′,3′-Di-Me ether: [74174-29-1]. *4′,7-Dihydroxy-2′,3′-dimethoxyisoflavene.* ***Haginin A***
$C_{17}H_{16}O_5$ M 300.310
Isol. from *L. cyrtobotrya* heartwood. Needles (MeOH/C_6H_6). Mp 130.5-131.5°.

2′,4′-Di-Me ether: [62078-14-2]. *3′,7-Dihydroxy-2′,4′-dimethoxyisoflavene.* ***2′-O-Methylsepiol***
$C_{17}H_{16}O_5$ M 300.310
Isol. from *G. sepium* heartwood. Oil. Mp 104-105° (as diacetate).

Tetra-Me ether: Mp 102-103°.

Jurd, L. *et al*, *J. Agric. Food Chem.*, 1977, **25**, 723 (*Sepiol*, 2-*O*-Methylsepiol)
Miyase, T. *et al*, *Chem. Pharm. Bull.*, 1980, **28**, 1172; 1981, **29**, 2205 (*Haginins*)

2′,4′,7,8-Tetrahydroxyisoflavene T-80104



$C_{15}H_{12}O_5$ M 272.257

4′,8-Di-Me ether: 2′,7-Dihydroxy-4′,8-dimethoxyisoflavene
$C_{17}H_{16}O_5$ M 300.310
Constit. of *Centrolobium* spp. Cryst. ($CHCl_3$). Mp 160-161°.

Alegrio, L.V. *et al*, *Phytochemistry*, 1989, **28**, 2359 (*isol, pmr, cmr*)

2′,3′,4′,7-Tetrahydroxyisoflavone T-80105

Updated Entry replacing T-03371

7-Hydroxy-3-(2,3,4-trihydroxyphenyl)-4H-1-benzopyran-4-one

$C_{15}H_{10}O_6$ M 286.240

4′-Me ether: [65048-75-1]. *2′,3′,7-Trihydroxy-4′-methoxyisoflavone.* ***Koparin***
$C_{16}H_{12}O_6$ M 300.267
Constit. of the wood of *Castanospermum australe*. Needles (EtOH). Mp 269-271°.

3′,4′,7-Tri-Me ether: [71973-12-1]. *2′-Hydroxy-3′,4′,7-trimethoxyisoflavone*

$C_{18}H_{16}O_6$ M 328.321
Isol. from trunkwood of *Myroxylon peruiferum*. Mp 210-212°.

3′,4′-Methylenedioxy ether: [65242-64-0]. *2′,7-Dihydroxy-3′,4′-methylenedioxyisoflavone.* ***Glyzaglabrin***
$C_{16}H_{10}O_6$ M 298.251
Isol. from root of *Glycyrrhiza glabra*.

Berry, R.C. *et al*, *Aust. J. Chem.*, 1977, **30**, 1827 (*Koparin*)
Bhardwaj, D.K. *et al*, *Curr. Sci.*, 1977, **46**, 753 (*Glyzaglabrin*)
Maranduba, A.A. *et al*, *Phytochemistry*, 1979, **18**, 815 (*2′-Hydroxy-3′,4′,7-trimethoxyisoflavone*)

2′,4′,5,7-Tetrahydroxyisoflavone T-80106

Updated Entry replacing T-40080

*3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. 2′-Hydroxygenistein*

[1156-78-1]

$C_{15}H_{10}O_6$ M 286.240
Isol. from *Apios tuberosa, Argyrocytisus battandieri, Cajanus cajan, Crotalaria juncea, Dolichos biflorus, Hardenbergia violacea, Lablab niger, Laburnium anagyroides, Lupinus albus, Moghania macrophylla, Neotonia wightii, Phaseolus vulgaris, P. coccineus, Spartium junceum* and *Stizolobium deeringianum* (all Leguminosae, Papilionoideae). Cryst. ($CHCl_3$/MeOH). Mp 270-273°.

4′-Me ether: [32884-35-8]. *2′,5,7-Trihydroxy-4′-methoxyisoflavone. Dehydroferreirin. 2′-Hydroxybiochanin A*
$C_{16}H_{12}O_6$ M 300.267
Isol. from *Virola caducifolia, V. multinervia* and *Haplormosia monophylla*. Needles (MeOH aq.). Mp 215-216° (201-203°).

5-Me ether: [58115-29-0]. *2′,4′,7-Trihydroxy-5-methoxyisoflavone. 2′-Hydroxyisoprunetin*
$C_{16}H_{12}O_6$ M 300.267
Constit. of *P. coccineus*.

7-Me ether: [32884-36-9]. *2′,4′,5-Trihydroxy-7-methoxyisoflavone.* ***Cajanin***
$C_{16}H_{12}O_6$ M 300.267
Isol. from *Cajanus cajan, Canavalia ensiformis, Centrosema pascuorum* and *C. pubescens*.

2′,4′-Di-Me ether: [61243-75-2]. *5,7-Dihydroxy-2′,4′-dimethoxyisoflavone. 2′-Methoxybiochanin A*
$C_{17}H_{14}O_6$ M 314.294
Constit. of *V. caducifolia* and *V. multinervia*. Cryst. (MeOH). Mp 222-223°.

2′,5-Di-Me ether: 4′,7-Dihydroxy-2′,5-dimethoxyisoflavone
$C_{17}H_{14}O_6$ M 314.294
From *P. coccineus*.

Farkas, L. *et al*, *J. Chem. Soc. C*, 1971, **10**, 1994 (*synth*)
Braz Filho, R. *et al*, *Phytochemistry*, 1976, **15**, 1029 (*isol, uv, ir, pmr, ms, derivs*)
Ingham, J.L., *Z. Naturforsch., C*, 1976, **31**, 504; 1977, **32**, 1018 (*isol*)
Prasad, J.S. *et al*, *Phytochemistry*, 1977, **16**, 1120 (*isol, uv, pmr, struct*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Adeesanya, S.A. *et al*, *Phytochemistry*, 1985, **24**, 2699 (*isol, derivs*)

2′,4′,5′,7-Tetrahydroxyisoflavone T-80107

Updated Entry replacing T-30093

$C_{15}H_{10}O_6$ M 286.240

2′,4′,5′-Tri-Me ether: [29096-94-4]. *7-Hydroxy-2′,4′,5′-trimethoxyisoflavone*
$C_{18}H_{16}O_6$ M 328.321
Constit. of *Eysenhardtia polystachya*. Also from *Amorpha fruticosa* and *Dalbergia monetaria*. Reputed to be the substance in Robert Boyle's fluorescent acid-base indicator used in the seventeenth century. Cryst. ($CHCl_3$). Mp 244-245° (234-237°).

2′-Me, 4′,5′-methylene ether: [7741-28-8]. *7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavone.* ***Cuneatin.*** *Maximaisoflavone G*
$C_{17}H_{12}O_6$ M 312.278
Constit. of *Tephrosia maxima* and *Cicer cuneatum*. Cryst. (MeOH). Mp 298-302°.

2′,7-Di-Me, 4′,5′-methylene ether: [4253-00-3]. *2′,7-Dimethoxy-4′,5′-methylenedioxyisoflavone. Cuneatin methyl ether*
$C_{18}H_{14}O_6$ M 326.305
Isol. from *Pterodon apparicioi* trunkwood. Prisms. Mp 210-212°.

Tetra-Me ether: [4253-02-5]. *2′,4′,5′,7-Tetramethoxyisoflavone*
$C_{19}H_{18}O_6$ M 342.348
Isol. from *Amorpha fruticosa* fruit and *Calopogonium mucunoides* seeds. Cryst. Mp 193-194°.

2′-Me, 4′,5′-methylene ether, 7-O-(3-methyl-2-butenyl): ***Maximaisoflavone C.*** *Maximin*
$C_{22}H_{20}O_6$ M 380.396
Isol. from *T. maxima* pods and roots. Prisms (Me_2CO). Mp 142-144°.

Rangaswami, S. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1959, **292**, 170 (*Maximaisoflavone C*)
Fukui, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1963, **36**, 397 (*synth*)
Galina, E. *et al*, *Phytochemistry*, 1974, **13**, 2593 (*Cuneatin methyl ether*)
Ognyanov, I. *et al*, *Planta Med.*, 1980, **38**, 279 (*2′,4′,5′,7-Tetramethoxyisoflavone*)
Rao, E.V. *et al*, *Phytochemistry*, 1984, **23**, 1493 (*isol*)
Burns, D.T. *et al*, *Phytochemistry*, 1984, **23**, 167 (*isol, struct*)

2′,5,6,7-Tetrahydroxyisoflavone T-80108

$C_{15}H_{10}O_6$ M 286.240

5-Me,6,7-methylene ether: [51068-94-1]. *2′-Hydroxy-5-methoxy-6,7-methylenedioxyisoflavone.* ***Betavulgarin***
$C_{17}H_{12}O_6$ M 312.278
Isol. from several *Beta* spp. and *Dianthus* spp. as phytoalexin. Shows strong antifungal activity. Cryst. solid. Mp 147-150°.

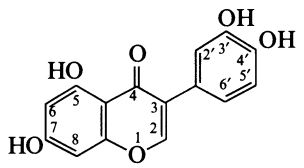
Geigert, J. *et al*, *Tetrahedron*, 1973, **29**, 2703 (*isol, uv, pmr, struct*)

3′,4′,5,7-Tetrahydroxyisoflavone T-80109

Updated Entry replacing T-60108

Orobol. *Norsantal*

[480-23-9]



$C_{15}H_{10}O_6$ M 286.240
Isol. from *Baptisa* spp., *Bolusanthus speciosus, Cytisus scoparius, Lathyrus* spp. and *Thermopsis* spp. (Leguminosae, Papilionoideae). Also prod. by microorganisms *Aspergillis niger, Fusarium, Stemphylium* and *Streptomyces* spp. Pale-yellow cryst. (AcOH). Mp 212°. All isolations of isoflavonoids from microorganisms are considered doubtful.

Tetra-Ac: [1061-93-4].

Cryst. (AcOH). Mp 212°.

7-O-Glucoside: [20486-33-3]. ***Oroboside***
$C_{21}H_{20}O_{11}$ M 448.382
Isol. from *Baptisia* spp., *Thermopsis* spp., *Lathyrus macrorrhizus* and *L. montanus*. The struct. of Oroboside as the 7-glucoside is not confirmed.

7-O-Rhamnosyglucoside: Orobol rhamnosylglucoside
$C_{27}H_{30}O_{15}$ M 594.525
Isol. from *B.* spp. λ_{max} 219, 259, 286sh, 330sh nm (MeOH).

3′-Me ether: [36190-95-1]. *4′,5,7-Trihydroxy-3′-methoxyisoflavone. 3′-O-Methylorobol*
$C_{16}H_{12}O_6$ M 300.267
Isol. from *Dalbergia inundata, Wyethia helenoides, W. mollis* and *Thermopsis* spp. Cryst. (MeOH). Mp 218-222°.

3′-Me ether, 7-O-glucoside:
$C_{22}H_{22}O_{11}$ M 462.409
Present in *Thermopsis* spp.

4′-Me ether: [2284-31-3]. *3′,5,7-Trihydroxy-4′-methoxyisoflavone.* ***Pratensein***
$C_{16}H_{12}O_6$ M 300.267
Constit. of *Bolusanthus speciosus, Trifolium* spp., *Cicer arietinum, Cytisus scoparius, Monopteryx inpae, Sophora japonica* and *Thermopsis* spp. Cryst. (EtOH). Mp 272-273°.

4′-Me ether, 7-O-glucoside: Pratensein 7-O-glucoside
$C_{22}H_{22}O_{11}$ M 462.409
Present in *Thermopsis* and *Trifolium* spp.

7-Me ether: [529-60-2]. *3′,4′,5-Trihydroxy-7-methoxyisoflavone.* ***Santal***
$C_{16}H_{12}O_6$ M 300.267
Constit. of *Pterocarpus osun* and *P. soyauxi*, also *Baphia nitida, W. helenoides* and *W. mollis*. Cryst. (EtOH). Mp 222-223°.

7-Me ether, tri-Ac: Cryst. (C_6H_6). Mp 147°.

3′,4′-Di-Me ether: 5,7-Dihydroxy-3′,4′-dimethoxyisoflavone. 3′-O-Methylpratensein
$C_{17}H_{14}O_6$ M 314.294
Constit. of *B. speciosus*.

3′,7-Di-Me ether: 4′,5-Dihydroxy-3′,7-dimethoxyisoflavone
$C_{17}H_{14}O_6$ M 314.294
Constit. of *P. soyauxii*.

3′,7-Di-Me ether, 4′,5-Di-Ac: Cryst. (EtOH). Mp 179°.

5,7-Di-Me, 3′,4′-bis(3-methyl-2-butenyl) ether: [65893-94-9]. ***Glabrescione B.*** *5,7-Dimethoxy-3′,4′-diprenyloxyisoflavone*
$C_{27}H_{30}O_6$ M 450.530
Isol. from seeds of *D. glabrescens*. Cryst. (CH_2Cl_2/heptane). Mp 102-104°.

3′,4′-Methylene ether: 5,7-Dihydroxy-3′,4′-methylenedioxyisoflavone. 3′,4′-Methylenedioxyorobol. 5-Hydroxypseudobaptigenin
$C_{16}H_{10}O_6$ M 298.251
Isol. from *Lupinus luteus* and *Sophora japonica*.

3′,4′-Methylene ether, 7-O-glucoside:
$C_{22}H_{20}O_{11}$ M 460.393
Isol. from *Lupinus angustfolius, L. luteus* and *L. polyphyllus*.

3′,4′-Methylene ether, 7-O-glucosylglucoside:
$C_{28}H_{30}O_{16}$ M 622.535
Isol. from roots of *L. luteus*.

5,7-Di-Me, 3′,4′-methylenedioxy ether: [22044-59-3]. *5,7-Dimethoxy-3′,4′-methylenedioxyisoflavone.* ***Derrustone***
$C_{18}H_{14}O_6$ M 326.305
Isol. from *Derris robusta* roots. Needles (MeOH). Mp 153-154°.

Akisanya, A. *et al, J. Chem. Soc.*, 1959, 2679 (*isol*)
Wong, E. *et al, J. Org. Chem.*, 1963, **28**, 2336 (*isol, struct, synth*)
Markham, K.R. *et al, Phytochemistry*, 1968, **7**, 791 (*isol*)
Dement, A.W. *et al, Phytochemistry*, 1972, **11**, 1089 (*isol*)
Adinarayana, D. *et al, Indian J. Chem.*, 1974, **12**, 911 (*synth*)
Laman, N.A. *et al, Khim. Prir. Soedin.*, 1974, 162; *cnc*, 175 (*3′,4′-Methylenedioxyorobol*)
Leite de Almeida, M.E. *et al, Phytochemistry*, 1974, **13**, 751 (*isol*)
Delle Monache, F. *et al, Gazz. Chim. Ital.*, 1977, **107**, 403 (*Glabrescione B*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Asnes, K. *et al, Z. Naturforsch., C*, 1985, **40**, 617 (*isol*)
Jain, A.C. *et al, Indian J. Chem., Sect. B*, 1987, **26**, 488 (*synth*)
Bezuidenhoudt, B.C.B. *et al, Phytochemistry*, 1987, **26**, 531 (*isol*)

3′,4′,5′,7-Tetrahydroxyisoflavone T-80110

*7-Hydroxy-3-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Baptigenin***

[5908-63-4]

$C_{15}H_{10}O_6$ M 286.240
Isol. from roots of *Baptisia tinctoria*. Cryst. (EtOH). Mp 284-285° (278-284°). Sublimes.

Tetra-Ac: Mp 214°.

O-*Rhamnoside:* ***Baptisin***
$C_{21}H_{20}O_{10}$ M 432.383
Isol. from root of *B. tinctoria*. Cryst. (EtOH aq.). Mp 240° (sinters from 150°).

4′-Me ether: [72061-64-4]. *3′,5′,7-Trihydroxy-4′-methoxyisoflavone.* ***Gliricidin***
$C_{16}H_{12}O_6$ M 300.267
Isol. from heartwood of *Gliricidia sepium*. Prisms (MeOH aq.). Mp 298° dec.

Tetra-Me ether: 3′,4′,5′,7-Tetramethoxyisoflavone
$C_{19}H_{18}O_6$ M 342.348
Cryst. (MeOH). Mp 144.5°.

Farkas, L. *et al, Chem. Ber.*, 1963, **96**, 1865 (*struct, bibl*)
Manners, G.D. *et al, Phytochemistry*, 1979, **18**, 1037 (*Gliricidin*)

3′,4′,6,7-Tetrahydroxyisoflavone T-80111

Updated Entry replacing H-20254

*3-(3,4-Dihydroxyphenyl)-6,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI*

4′,6-Di-Me ether: [53948-00-8]. *3′,7-Dihydroxy-4′,6-dimethoxyisoflavone.* ***Odoratin***†
$C_{17}H_{14}O_6$ M 314.294
Isol. from *Dipteryx odorata* heartwood and *Pterodon apparicioi* trunkwood. There are at least three other odoratins.

4′,6-Di-Me ether, di-Ac: Needles (MeOH). Mp 210-211°.

3′,4′,6-Tri-Me ether: [24126-90-7]. *7-Hydroxy-3′,4′,6-trimethoxyisoflavone.* ***Cladrastin***
$C_{18}H_{16}O_6$ M 328.321
Isol. from *Cladrastis lutea, C. platycarpa* and *C. shikokiana*. Mp 206-207°.

3′,4′,6-Tri-Me ether, 7-O-β-D-glucopyranoside: [59183-50-5].
$C_{24}H_{26}O_{11}$ M 490.463
Isol. from *C. platycarpa* and *C. shikokiana*. Mp 213-215°.

3′,4′,6-Tri-Me ether, O-*laminaribioside:*
$C_{30}H_{36}O_{16}$ M 652.605
Isol. from *C. platycarpa* and *C. shikokiana*.

6-Me, 3′,4′-methylenedioxy ether: [38965-66-1]. *7-Hydroxy-6-methoxy-3′,4′-methylenedioxyisoflavone.* ***Fujikinetin***
$C_{17}H_{12}O_6$ M 312.278
Isol. from *C. platycarpa, C. shikokiana, Dalbergia riparia, D. sericea* and *P. apparicioi*. Mp 279-281° dec.

6-Me, 3′,4′-methylenedioxy ether, 7-O-β-D-glucopyranoside: [38965-67-2]. ***Fujikinin***
$C_{23}H_{22}O_{11}$ M 474.420
Constit. of *C. platycarpa* and *C. shikokiana*. Mp 155-160°.

Tetra-Me ether: 3′,4′,6,7-Tetramethoxyisoflavone
$C_{19}H_{18}O_6$ M 342.348
Isol. from *Cordyla africana*, *P. apparicioi* and *P. pubsescens*. Laths (MeOH). Mp 187-188°.

3′,4′-Di-Me, 6,7-methylenedioxy ether: [2746-85-2]. *3′,4′-Dimethoxy-6,7-methylenedioxyisoflavone*
$C_{18}H_{14}O_6$ M 326.305
Isol from heartwood of *Xanthocercis zambesiaca*. Microcryst. ($CHCl_3$/pet. ether). Mp 258-259°.

6-Me, 3′,4′-methylenedioxy ether, 7-O-laminarabioside:
$C_{29}H_{32}O_{16}$ M 636.562
Isol. from *Cladrastis platycarpa* and *C. shikokiana*.

6,7-Di-Me, 3′,4′-methylenedioxy ether: [55303-89-4]. *6,7-Dimethoxy-3′,4′-methylenedioxyisoflavone.* ***Milletenin C.*** *Fujikinetin methyl ether*
$C_{18}H_{14}O_6$ M 326.305
Isol. from heartwood of *Cordyla africana* and from *Milletia ovalifolia*. Needles (EtOH). Mp 252-253° (245-246°).

Shamma, M. *et al*, *Tetrahedron*, 1965, **25**, 3887 (*Cladrastin*)
Campbell, R.V.M. *et al*, *J. Chem. Soc. C*, 1969, 1787 (*isol*)
Hayashi, T. *et al*, *Phytochemistry*, 1974, **13**, 1943 (*Odoratin*)
Khan, H. *et al*, *Tetrahedron*, 1974, **30**, 2811 (*Milletenin C*)
Antus, S. *et al*, *Chem. Ber.*, 1975, **108**, 3883 (*synth*)
de Almeida, M.E.L., *Phytochemistry*, 1975, **14**, 2716 (*isol*)
Harper, S.H. *et al*, *Phytochemistry*, 1976, **15**, 1019 (3,′4′-*Dimethoxy-6,7-methylenedioxyisoflavone*)
Ohashi, H. *et al*, *Phytochemistry*, 1976, **15**, 354 (*Cladrastin*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*occur*)

4′,5,6,7-Tetrahydroxyisoflavone T-80112

Updated Entry replacing D-30313

5,6,7-Trihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 6-Hydroxygenistein
$C_{15}H_{10}O_6$ M 286.240
Isol. from *Baptisia hirsuta* and *Centrosema plumieri*. Fawn cryst. (EtOAc). Mp 243-250° dec.

7-O-Rhamnosylglucside:
$C_{27}H_{30}O_{15}$ M 594.525
Isol. from leaves and stems of *Baptisia hisuta*. λ_{max} 269, 340sh nm (MeOH).

6-Me ether: see 4′,5,7-*Trihydroxy-6-methoxyisoflavone*, *T-80319*

4′,6-Di-Me ether: [2345-17-7]. *5,7-Dihydroxy-4′,6-dimethoxyisoflavone.* ***Irisolidone.*** *4′-O-Methyltectorigenin*
$C_{17}H_{14}O_6$ M 314.294
Constit. of *Podocarpus amarus* and *Iris* spp. Also *Pericopsis mooniana*, *Pueraria thunbergiana* and *Sophora japonica*. Cryst. (EtOH). Mp 200-203° (189-190°).

4′,6-Di-Me ether, 7-β-D-glucopyranoside: ***Kakkalidone***
$C_{23}H_{24}O_{11}$ M 476.436
Constit. of *I. germanica*, *Pueraria thunbergiana* and *S. japonica*. Amorph. powder (MeOH). Mp 215-216°.

4′-Di-Me ether, 7-O-[β-D-xylopyranosyl(1→6)β-D-glucopyranoside]: [58274-56-9]. ***Kakkalide***
$C_{28}H_{32}O_{15}$ M 608.552
Isol. from flowers of *P. thunbergiana*. Tetrahydrate. Mp 253°. $[\alpha]_D^{24}$ −31° (c, 1.0 in Py).

5,7-Di-Me ether: [479-83-4]. *4′-6-Dihydroxy-5,7-dimethoxyisoflavone.* ***Muningin***
$C_{17}H_{14}O_6$ M 314.294
Isol. from *Podocarpus angolensis*, heartwood. Cryst. + $\frac{1}{2}H_2O$ (dioxan). Mp 285° dec.

6,7-Di-Me ether: [1096-58-8]. *4′,5-Dihydroxy-6,7-dimethoxyisoflavone. 7-O-Methyltectorigenin*
$C_{17}H_{14}O_6$ M 314.294
Isol. from *Dalbergia sissoo*, *D. spruceana*, *D. volubilis* and *Pterocarpus angolensis*. Pale-yellow needles (MeOH). Mp 235-236° (228-229°).

6,7-Di-Me ether, 4′-O-glucoside:
$C_{23}H_{24}O_{11}$ M 476.436
Isol. from bark of *Dalbergia volubilis*. Mp 130-133°. $[\alpha]_D$ −16.32° (c, 0.68 in MeOH).

6,7-Di-Me ether, 4′-O-rhamnosylglucoside:
$C_{29}H_{24}O_{15}$ M 612.500
Isol. from immature pods of *D. sissoo*.

6,7-Di-Me ether, 4′-O-[4-O-β-D-glucopyranosyl (1→4)-β-D-glucopyranoside]:
$C_{29}H_{34}O_{16}$ M 638.578
Isol. from bark of *D. volubilis*. Mp 180-183°. $[\alpha]_D$ −21° (c, 0.75 in Py).

4′,5,6-Tri-Me ether: 7-Hydroxy-4′,5,6-trimethoxyisoflavone. 5-Methoxyafrormosin
$C_{18}H_{16}O_6$ M 328.321
Isol. from *Cladrastis platycarpa*, *C. shikokiana* and *Wisteria floribunda*.

4′,6,7-Tri-Me ether: 5-Hydroxy-4′,6,7-trimethoxyisoflavone. 4′,7-Di-O-methyltectorigenin
$C_{18}H_{16}O_6$ M 328.321
Isol. from flowers of *Dalbergia sissoo*. Mp 189-190°.

6,7-Methylenedioxy ether: see 4′,5-*Dihydroxy-6,7-methylenedioxyisoflavone*, *D-80341*

4′,5,6-Tri-Me ether, 7-O-glucoside:
$C_{24}H_{26}O_{11}$ M 490.463
Isol. from *C. platycarpa* and *C. shikokiana*.

4′,5,6-Tri-Me ether, 7-O-Laminarabioside: Isol. from *C. platycarpa* and *C. shikokiana*. Tentative struct.

King, F.E. *et al*, *J. Chem. Soc.*, 1952, 96 (*Muningin*)
Prakash, L. *et al*, *J. Org. Chem.*, 1965, **30**, 3561 (*isol*, *deriv*)
Markham, K.R. *et al*, *Phytochemistry*, 1968, **7**, 803; 1970, **9**, 2359 (*isol*, *uv*)
Dhar, K.L. *et al*, *J. Indian Chem. Soc.*, 1975, **52**, 784 (*isol*, *uv*, *ir*, *nmr*, *Irisolidone*)
Kurihara, T. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1975, **95**, 1283 (*Kakkalide*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev*, *occur*)
Ali, A.A. *et al*, *Phytochemistry*, 1983, **22**, 2061 (*isol*)
Carman, R.M. *et al*, *Aust. J. Chem.*, 1985, **38**, 485.

4′,5,7,8-Tetrahydroxyisoflavone T-80113

Updated Entry replacing T-03377

5,7,8-Trihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI

[13539-27-0]

$C_{15}H_{10}O_6$ M 286.240
Metab. of *Aspergillus niger*. All isolations of isoflavones from microorganisms are considered suspect.

8-Me ether: [13111-57-4]. *4′,5,7-Trihydroxy-8-methoxyisoflavone.* ***Isotectorigenin.*** *Pseudotectorigenin*
$C_{16}H_{12}O_6$ M 300.267
Isol. from *Dalbergia sissoo* bark, *Millettia auriculata* seeds and metab. of *A. niger*. DOPA decarboxylase inhibitor. Pale yellow needles (MeOH). Mp 245°.

4′,5,8-Tri-Me ether: [68862-20-4]. *7-Hydroxy-4′,5,8-trimethoxyisoflavone. Iso-5-methoxyafrormosin*
$C_{18}H_{16}O_6$ M 328.321

Isol. from *Cladrastis platycarpa* and *C. shikokiana*. Tentative identification.

4′,5,8-Tri-Me ether, 7-O-β-D-glucoside:
$C_{24}H_{26}O_{11}$ M 490.463
Isol. from *C. platycarpa* and *C. shikokiana*.

8-O-Me, 4′-O-(3-methyl-2-butenyl): [68415-32-7]. ***Aurmillone***
$C_{21}H_{20}O_6$ M 368.385
Constit. of *Millettia auriculata*. Mp 157-158°.

Dhingra, V.K. *et al*, *Indian J. Chem.*, 1974, **12**, 1118 (*Isotectorigenin*)
Umezawa, H. *et al*, *J. Antibiot.*, 1975, **28**, 947 (*isol*)
Ohashi, H. *et al*, *Mokuzai Gakkaishi*, 1978, **24**, 750; *CA*, **90**, 36297z (*isol*)
Srimannarayana, G. *et al*, *Phytochemistry*, 1978, **17**, 1065 (*Aurmillone*)

1,2,5,7-Tetrahydroxyphenanthrene T-80114

Updated Entry replacing T-60116

1,2,5,7-Phenanthrenetetrol
$C_{14}H_{10}O_4$ M 242.231

1,5-Di-Me ether: [86630-47-9]. *1,5-Dimethoxy-2,7-phenanthrenediol. 2,7-Dihydroxy-1,5-dimethoxyphenanthrene*
$C_{16}H_{14}O_4$ M 270.284
Constit. of *Oncidium cebolleta* and *Eulophia nuda*. Magenta needles ($CHCl_3$/MeOH). Mp 200-201°.

Tetra-Me ether: [96754-01-7]. *1,2,5,7-Tetramethoxyphenanthrene*
$C_{18}H_{18}O_4$ M 298.338
Cryst. (EtOAc/hexane). Mp 134°.

9,10-Dihydro, 2,7-Di-Me ether: [87402-72-0]. *9,10-Dihydro-2,7-dimethoxy-1,5-phenanthrenediol, 9CI.* 9,10-*Dihydro-*1,5-*dihydroxy-*2,7-*dimethoxyphenanthrene.* ***Eulophiol***
$C_{16}H_{16}O_4$ M 272.300
Constit. of *Eulophia nuda* tubers. Cryst. ($CHCl_3$). Mp 202-203°.

9,10-Dihydro, 2,5-di-Me ether: 9,10-Dihydro-2,5-dimethoxy-1,7-phenanthrenediol. 9,10-Dihydro-1,7-dihydroxy-2,5-dimethoxyphenanthrene
$C_{16}H_{16}O_4$ M 272.300
Constit. of *E. nuda*. Needles ($CHCl_3$/MeOH). Mp 202-203°. Shown to be not identical with eulophiol even though the melting points are the same.

Stermitz, F.R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1983, **46**, 417 (*isol*)
Bhandari, S.R. *et al*, *Phytochemistry*, 1983, **22**, 747 (*isol*)
Bhandari, S.R. *et al*, *Indian J. Chem.*, *Sect. B*, 1985, **24**, 204 (*synth, deriv, uv, pmr*)
Tuchinda, P. *et al*, *Phytochemistry*, 1988, **27**, 3267 (*isol, cryst struct*)

2,3,4,7-Tetrahydroxyphenanthrene T-80115

Updated Entry replacing T-50177

2,3,4,7-Phenanthrenetetrol
$C_{14}H_{10}O_4$ M 242.231

2,4-Di-Me ether: [72966-94-0]. *5,7-Dimethoxy-2,6-phenanthrenediol. 3,7-Dihydroxy-2,4-dimethoxyphenanthrene*
$C_{16}H_{14}O_4$ M 270.284
Constit. of *Eulophia nuda*. Prisms. Mp 185°.

2,4-Di-Me ether, di-Ac: Needles ($CHCl_3$/hexane). Mp 144-145°.

3,4-Di-Me ether: [86630-46-8]. *3,4-Dimethoxy-2,7-phenanthrenediol. 2,7-Dihydroxy-3,4-dimethoxyphenanthrene.* ***Nudol***
$C_{16}H_{14}O_4$ M 270.284
Constit. of *Oncidium cebolleta* and of *Eulophia* spp.

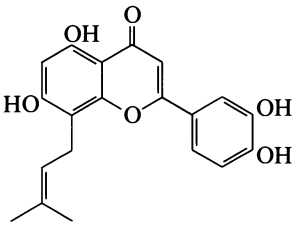
3,4-Di-Me ether, 2,7-Di-Ac: Cryst. Mp 159° (156°).

3,4-Di-Me ether, 9,10-dihydro: [101508-48-9]. *9,10-Dihydro-3,4-dimethoxy-2,7-phenanthrenediol. 9,10-Dihydro-2,7-dihydroxy-3,4-dimethoxyphenanthrene.* ***Erianthridin***
$C_{16}H_{16}O_4$ M 272.300
Constit. of *Eria carinata* and *E. stricta*. Amorph.

Stermitz, F.R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1983, **46**, 417 (*isol*)
Majumder, P.L. *et al*, *Indian J. Chem.*, *Sect. B*, 1985, **24**, 1192 (*Erianthridin*)
Bhandari, S.R. *et al*, *Phytochemistry*, 1985, **24**, 801 (*Nudol*)
Tuchinda, P. *et al*, *Phytochemistry*, 1988, **27**, 3267 (*isol*)

3′,4′,5,7-Tetrahydroxy-8-prenylflavone T-80116

*2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one*
[14926-12-6]

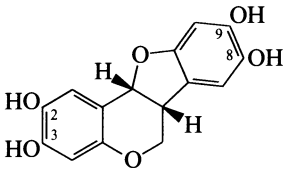


$C_{20}H_{18}O_6$ M 354.359
Isol. from *Xanthium spinosum* and *X. strumarium*. Mp 209-211°.

Pashchenko, M.M. *et al*, *CA*, 1966, **65**, 5871f; **66**, 49239m.

2,3,8,9-Tetrahydroxypterocarpan T-80117

Updated Entry replacing H-02198



$C_{15}H_{12}O_6$ M 288.256

3,9-Di-Me ether: [76474-65-2]. *2,8-Dihydroxy-3,9-dimethoxypterocarpan*
Isol. from *Swartzia laevicarpa*. Cryst. (C_6H_6/pet. ether). Mp 178-180°.

3-Me, 8,9-methylenedioxy ether: [30461-92-8]. *2-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan. 2-Hydroxypterocarpin*
$C_{17}H_{14}O_6$ M 314.294
Constit. of *Neorautanenia edulis* and *S. leiocalycina*. Needles (Me_2CO). Mp 238-239°. $[\alpha]_D^{23}$ −227.7° (c, 0.8 in $CHCl_3$).

2,3-Di-Me, 8,9-methylene ether: [30461-93-9]. *2,3-Dimethoxy-8,9-methylenedioxypterocarpan. 2-Methoxypterocarpin*
$C_{18}H_{16}O_6$ M 328.321
Isol. from root bark of *N. edulis*. Prisms. Mp 163.8°. $[\alpha]_D^{25}$ −231.8° (c, 1.3 in $CHCl_3$).

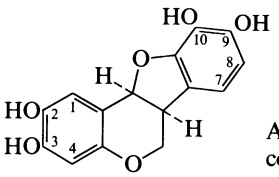
(±)-form

3-Me, 8,9-methylenedioxy ether: [52305-02-9]. Needles (Me_2O). Mp 223-224°.

Rall, G.J.H. *et al*, *Tetrahedron*, 1970, **26**, 5007 (*2-Hydroxypterocarpin, abs config*)
Rall, G.J.H. *et al*, *J. S. Afr. Chem. Inst.*, 1972, **25**, 25 (*2-Methoxypterocarpin*)

Farkas, L. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1974, 305 (*synth*)
Braz Filho, R. *et al*, *Phytochemistry*, 1980, **19**, 2003 (2,8-*Dihydroxy*-3,9-*dimethoxypterocarpan*)

2,3,9,10-Tetrahydroxypterocarpan T-80118



Absolute configuration

$C_{15}H_{12}O_6$ M 288.256

3,9-Di-Me ether: [69743-89-1]. *2,10-Dihydroxy-3,9-dimethoxypterocarpan.* ***Mucronucarpan***
$C_{17}H_{16}O_6$ M 316.310
Isol. from heartwood of *Machaerium mucronulatum*. Oil. $[\alpha]_D^{20}$ −15.4° (c, 0.42 in Me_2CO).

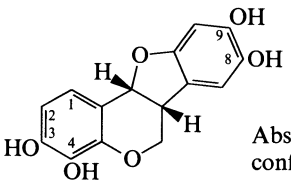
(±)-***form***

3,9-Di-Me ether: Needles (EtOH). Mp 173°.

Kurosawa, K. *et al*, *Phytochemistry*, 1978, **17**, 1405 (*isol, uv, pmr, ord, struct*)

3,4,8,9-Tetrahydroxypterocarpan T-80119

Updated Entry replacing H-02199



Absolute configuration

$C_{15}H_{12}O_6$ M 288.256

8,9-Methylene ether: 3,4-Dihydroxy-8,9-methylenedioxypterocarpan. 4-Hydroxymaackiain
$C_{16}H_{12}O_6$ M 300.267
Isol. from wood of *Dalbergia spruceana*. Cryst. (MeOH aq.). Mp 85-87°, Mp 186-187° (double Mp). $[\alpha]_D^{20}$ −233° (MeOH).

3-Me, 8,9-methylene ether: 4-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan. 4-Hydroxypterocarpin
$C_{17}H_{14}O_6$ M 314.294
Isol. from *D. spruceana* heartwood. Needles (MeOH), rhombs (pet. ether). Mp 172-174°. $[\alpha]_D^{20}$ −300° (MeOH).

4-Me, 8,9-methylene ether: [22973-31-5]. *3-Hydroxy-4-methoxy-8,9-methylenedioxypterocarpan. 4-Methoxymaackiain*
$C_{17}H_{14}O_6$ M 314.294
Constit. of *Amorpha californica, Baptisia australis, Dalbergia spruceana, Sophora franchetiana, Swartzia madagascariensis, Tephrosia bidwilli* and *Trifolium hybridum*. Needles (MeOH). Mp 159-161°. $[\alpha]_D$ −197° ($CHCl_3$).

3,4-Di-Me, 8,9-methylene ether: [2694-70-4]. *3,4-Dimethoxy-8,9-methylenedioxypterocarpan. 4-Methoxypterocarpin*
$C_{18}H_{16}O_6$ M 328.321
Isol. from tubers of *Neorantanenia ficifolia* and heartwood of *S. madagascariensis*. Prisms (C_6H_6). Mp 245-247°. $[\alpha]_D$ −202° ($CHCl_3$).

(±)-***form***

3,4-Di-Me, 8,9-methylene ether: Mp 226-227°.

Fukui, K. *et al*, *Experientia*, 1969, **25**, 122 (*synth, uv*)

Harper, S.H. *et al*, *J. Chem. Soc. C*, 1969, 1109 (*isol*)
Cook, J.T. *et al*, *Phytochemistry*, 1978, **17**, 1419 (*isol, uv, pmr, cd, struct*)

3,6*a*,7,9-Tetrahydroxypterocarpan T-80120

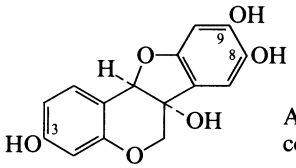
$C_{15}H_{12}O_6$ M 288.256

9-Me ether: [61135-98-6]. *3,6a,7-Trihydroxy-9-methoxypterocarpan. 6a,7-Dihydroxymedicarpin*
$C_{16}H_{14}O_6$ M 302.283
Isol. from leaves of *Melilotus alba* and *Trifolium pratense* as fungal metab. Not obt. pure.

Ingham, J.L., *Phytochemistry*, 1976, **15**, 1489 (*isol, uv*)

3,6*a*,8,9-Tetrahydroxypterocarpan T-80121

Updated Entry replacing P-20139



Absolute configuration

8,9-Methylenedioxy ether: [14602-93-8]. *3,6a-Dihydroxy-8,9-methylenedioxypterocarpan.* ***6a-Hydroxymaackiain.*** *6a-Hydroxyinermin*
Isol. from leaves of *Trifolium pratense* as fungal metab. Also prod. by cultures of *Ascochyta pisi, Botrytis cinerea, Fusarium* spp., *Nectria haematococca* and other fungi. Mp 178-181° dec. $[\alpha]_D^{21}$ +337° (c, 0.944 in EtOH).

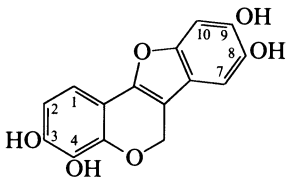
3-Me, 8,9-methylenedioxy ether: [20186-22-5]. *6a-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan.* ***Pisatin***
Stress metab. from *Caragana* spp., *Lathyrus* spp., *Pisum fulvum, P. sativum, Tephrosia bidwilli* and *Trifolium pratense*. Phytoalexin. Cryst. (EtOH or C_6H_6). Mp 61°. $[\alpha]_D^{20}$ +280° (c, 0.11 in EtOH).

(±)-***form***

3-Me, 8,9-methylenedioxy ether: Mp 188-190°.

Perrin, D.R. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 1919, 1922 (*isol*)
Bevan, C.W.L. *et al*, *J. Chem. Soc.*, 1964, 5991 (*synth*)
Fukui, K. *et al*, *Tetrahedron Lett.*, 1966, 1805 (*synth*)
Kelsey, T.C. *et al*, *Phytochemistry*, 1975, **14**, 1103 (*isol, struct*)
Bilton, J.N. *et al*, *Phytochemistry*, 1976, **15**, 1411 (*isol*)
de Martinis, C., *J. Cryst. Mol. Struct.*, 1978, **8**, 247 (*struct*)
Banks, S.W. *et al*, *Phytochemistry*, 1982, **21**, 1605, 2235; 1983, **22**, 1591 (*biosynth*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*occur*)

3,4,8,9-Tetrahydroxypterocarpene T-80122

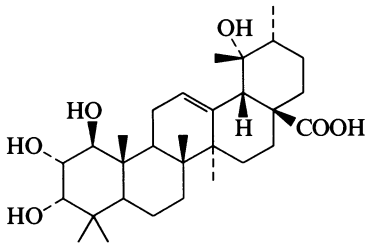


$C_{15}H_{10}O_6$ M 286.240

4-Me, 8,9-methylene ether: [56296-88-9]. ***3-Hydroxy-4-methoxy-8,9-methylenedioxypterocarpene***
$C_{17}H_{12}O_6$ M 312.278
Isol. from trunkwood of *Swartzia ulei*. Cryst. Mp 196-198°.

Formiga, M.D. *et al*, *Phytochemistry*, 1975, **14**, 828 (*isol, uv, ir, pmr, struct*)

1,2,3,19-Tetrahydroxy-12-ursen-28-oic acid T-80123



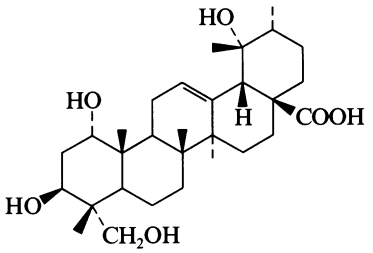
$C_{30}H_{48}O_6$ M 504.706

(1β,2α,3α,19α)-form

Constit. of *Rosa sterilis*. Amorph. solid. $[\alpha]_D$ +24° (c, 1.5 in EtOH).

Guang-Yi, L. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 162 (*isol*, *pmr*, *cmr*)

1,3,19,23-Tetrahydroxy-12-ursen-28-oic acid T-80124



$C_{30}H_{48}O_6$ M 504.706

(1α,3β,19α)-form

Cryst. Mp 270-272°.

O-β-D-Xylopyranosyl ester:

$C_{35}H_{56}O_{10}$ M 636.821

Constit. of *Centipeda minima*. Needles. Mp 139°.

2α-Hydroxy: 1α,2α,3β,19α,23-Pentahydroxy-12-ursen-28-oic acid

$C_{30}H_{48}O_7$ M 520.705

2α-Hydroxy, 28-β-D-xylopyranoside:

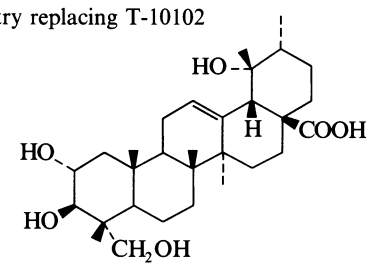
$C_{35}H_{56}O_{11}$ M 652.821

Constit. of *C. minina*. Cryst. Mp 210°.

Gupta, D. *et al*, *Phytochemistry*, 1989, **28**, 1197.

2,3,19,23-Tetrahydroxy-12-ursen-28-oic acid T-80125

Updated Entry replacing T-10102



$C_{30}H_{48}O_6$ M 504.706

(2α,3β,19α)-form [70868-78-9]

23-*Hydroxytormentic acid*

Constit. of *Epilobium hirsutum*.

Me ester:

$C_{31}H_{50}O_6$ M 518.732

Noncryst. $[\alpha]_D$ +14° (c, 0.6 in $CHCl_3$).

Me ester, 2,3,23-tri-Ac:

$C_{37}H_{56}O_9$ M 644.844

Cryst. (hexane). Mp 208-210°. $[\alpha]_D$ +20.1° (c, 0.9 in $CHCl_3$).

3,28-O-Bis-β-D-glucopyranosyl:

$C_{42}H_{68}O_{16}$ M 828.990

Constit. of *Symplocos spicata*. Needles (MeOH). Mp 236-239°. $[\alpha]_D$ +39° (c, 1.3 in MeOH).

β-D-Glucopyranosyl ester: Quercilicoside A

$C_{36}H_{58}O_{11}$ M 666.848

Constit. of *Quercus ilex*. Cryst. (EtOH aq.). Mp 247° dec.

28-O-β-D-Glucopyranoside: 23-Hydroxytormentic acid ester glucoside

$C_{36}H_{58}O_{11}$ M 666.848

Constit. of *Desfontainia spinosa*, *Geum japonicum* and *Aphloia theiformis*. Amorph. powder.

(2α,3α,19α)-form

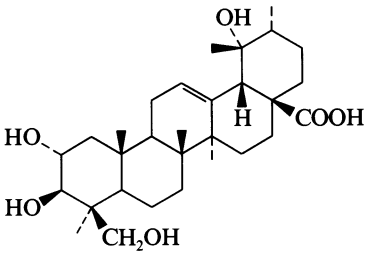
Myrianthic acid

Constit. of *Myrianthus arboreus* and *Coleus amboinicus*.

Me ester: Cryst. Mp 126°.

Teresa, J., de P. etal, *An. Quim.*, 1979, **75**, 135.
Higuchi, R. *et al*, *Phytochemistry*, 1982, **21**, 907.
Romussi, G. *et al*, *Justus Liebigs Ann. Chem.*, 1983, 1448.
Gopalsamy, N. *et al*, *Phytochemistry*, 1988, **27**, 3593 (*deriv*)
Kojima, H. *et al*, *Phytochemistry*, 1989, **28**, 1703 (*pmr*, *struct*)

2,3,19,24-Tetrahydroxy-12-ursen-28-oic acid T-80126



$C_{30}H_{48}O_6$ M 504.706

(2α,3α)-form

Constit. of *Rhododendron japonicum*.

Me ester: Amorph. powder. $[\alpha]_D^{21}$ +14.13° (c, 2.94 in MeOH).

(2α,3β)-form [105706-08-9] ***Hyptatic acid B.*** 24-*Hydroxytormentic acid*

Constit. of *Hyptis capitata* and *Desfontainia spinosa*. Amorph. powder. Mp 225-228°. $[\alpha]_D^{20}$ +28° (c, 0.2 in MeOH).

28-O-β-D-Glucopyranoside:

$C_{36}H_{58}O_{11}$ M 666.848

From *D. spinosa*. Amorph. solid.

Sakakibara, J. *et al*, *Phytochemistry*, 1983, **22**, 2547 (*isol*)
Houghton, P.J. *et al*, *Phytochemistry*, 1986, **25**, 1939 (*isol*)
Yamagishi, T. *et al*, *Phytochemistry*, 1988, **27**, 3213.
Kojima, H. *et al*, *Phytochemistry*, 1989, **28**, 1703 (*pmr*, *struct*)

2,3,6,19-Tetrahydroxy-12-ursen-28-oic acid T-80127

$C_{30}H_{48}O_6$ M 504.706

(2α,3β,6β,19α)-form [119528-66-4]

6β-*Hydroxytormentic acid*

Amorph. powder.

20-O-β-D-Glucopyranoside: [119513-60-9].

$C_{36}H_{58}O_{11}$ M 666.848
Constit. of *Aphoia theiformis*. Amorph. powder.

Gopalsamy, N. *et al*, *Phytochemistry*, 1988, **27**, 3593.

2,3,7,19-Tetrahydroxy-12-ursen-28-oic acid T-80128

Updated Entry replacing T-50183

$C_{30}H_{48}O_6$ M 504.706

(2α,3β,7α)-form

7α-Hydroxytormentic acid

Constit. of *Desfontainia spinosa*. Amorph. powder.

28-O-β-D-Glucopyranoside:

$C_{36}H_{58}O_{11}$ M 666.848

From *D. spinosa*. Amorph. powder.

(2α,3α,7β,19α)-form

Roxburic acid

Constit. of *Rosa roxburghii*.

Houghton, P.J. *et al*, *Phytochemistry*, 1986, **25**, 1939 (*isol*)
Kojima, H. *et al*, *Phytochemistry*, 1989, **28**, 1703 (*pmr*, *struct*)

3,6,19,23-Tetrahydroxy-12-ursen-28-oic acid T-80129

Updated Entry replacing T-30102

$C_{30}H_{48}O_6$ M 504.706

(3β,6β,19α)-form [91095-51-1]

Constit. of *Enkianthus campanulatus*.

23-Aldehyde: 3β,6β,19α-Trihydroxy-23-oxo-12-ursen-28-oic acid

$C_{30}H_{46}O_6$ M 502.690

Constit. of *Uncaria florida*.

23-Aldehyde, 3Ac, Me ester: Prisms. Mp 197-199°.

23-Carboxylic acid: 3β,6β,19α-Trihydroxy-12-ursene-23,28-dioic acid

$C_{30}H_{46}O_7$ M 518.689

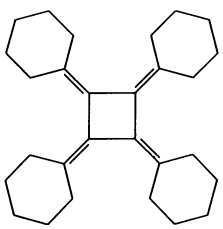
Constit. of *U. florida*.

Sakakibara, J. *et al*, *Phytochemistry*, 1984, **23**, 627 (*isol*)
Aimi, N. *et al*, *Tetrahedron*, 1989, **45**, 4125 (*isol*, *pmr*, *cmr*)

Tetrakis(cyclohexylidene)cyclobutane T-80130

1,1′,1″,1‴-(1,2,3,4-Cyclobutanetetraylidene)tetrakiscyclohexane, 9CI

[117471-48-4]

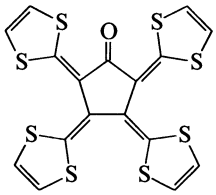


$C_{28}H_{40}$ M 376.624

Iyoda, M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 8494 (*synth*)

Tetrakis(1,3-dithiol-2-ylidene)cyclopentanone, 9CI T-80131

[112347-97-4]



$C_{17}H_8OS_8$ M 484.778

Electron donor with low oxidation potential. Reddish purple cryst. Mp 250° dec.

Sugimoto, T. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 628 (*synth*, *props*)

Tetrakis(trifluoromethylthio)ethene T-80132

$(F_3CS)_2C{=}C(SCF_3)_2$

$C_6F_{12}S_4$ M 428.311

Liq. Bp_8 49°. n_D^{25} 1.4253.

Harris, J.F., *J. Org. Chem.*, 1967, **32**, 2063 (*synth*, *uv*, *ir*)

Tetrakis(trifluoromethylthio)methane T-80133

Tetrathioorthocarbonic acid tetrakis(trifluoromethyl) ester, 8CI

[681-87-8]

$C(SCF_3)_4$

$C_5F_{12}S_4$ M 416.300

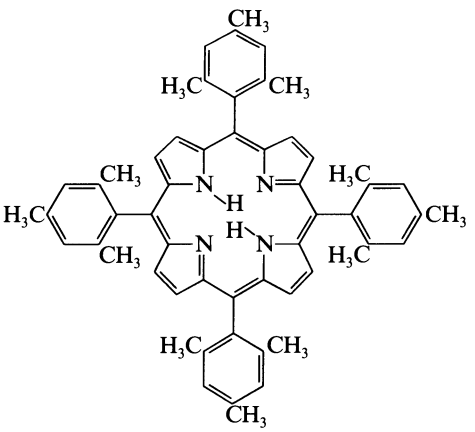
Bp_8 39-39.5°. n_D^{25} 1.4013.

Harris, J.F., *J. Org. Chem.*, 1967, **32**, 2063 (*synth*, *ir*, *uv*)

5,10,15,20-Tetrakis(2,4,6-trimethylphenyl)-21*H*,23*H*-porphine, 9CI T-80134

Tetramesitylporphyrin

[56396-12-4]



$C_{56}H_{54}N_4$ M 783.069

Synthetic sterically hindered model prophyrin. Purple needles (C_6H_6/MeOH).

Zn complex: [104025-54-9].

$C_{56}H_{52}N_4Zn$ M 846.444

Red-purple shiny cryst. ($CHCl_3$/hexane).

Ni complex: [109533-32-6].

Red-purple shiny cryst. ($CHCl_3$/hexane).

Pd complex: [109533-33-7].

Shiny purple cryst. (CH_2Cl_2/pentane).

Pt complex: [109533-34-8].
Red cryst. ($CHCl_3$/hexane).

Badger, G.M. *et al*, *Aust. J. Chem.*, 1964, **17**, 1028 (*synth*)
Eaton, S.S. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 3660 (*synth, nmr*)
Groves, J.T. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 6243 (*synth*)
Eberhardt, U. *et al*, *Justus Liebigs Ann. Chem.*, 1987, 809 (*synth, nmr, uv, complexes*)
Wagner, R.W. *et al*, *Tetrahedron Lett.*, 1987, **28**, 3069 (*synth, ir, uv, nmr*)

Tetramethoxyethene T-80135

Tetramethoxyethylene

$$(MeO)_2C{=}C(OMe)_2$$

$C_6H_{12}O_4$ M 148.158
Bp_{15} 48°. n_D^{20} 1.4244.

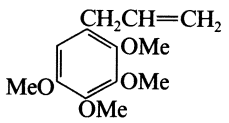
▷ Prepn. explosive on large scale.

Hoffmann, R.W. *et al*, *Tetrahedron*, 1965, **21**, 891 (*synth, pmr*)
Scheeren, J.W. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1973, **92**, 11 (*synth*)
Herberhold, M. *et al*, *Z. Naturforsch.*, *B*, 1976, **31**, 35 (*pmr, cmr*)
Kopecky, K.R. *et al*, *Can. J. Chem.*, 1988, **66**, 2234.

1,2,3,4-Tetramethoxy-5-(2-propenyl) benzene T-80136

1-Allyl-2,3,4,5-tetramethoxybenzene

[15361-99-6]



$C_{13}H_{18}O_4$ M 238.283
Isol. from parsley oil and other *Petroselinum* spp., and *Asarum* oils. Tablets (EtOH aq.). Mp 25°. Bp_{12} 145°.

Baker, W. *et al*, *J. Chem. Soc.*, 1934, 1681.
Shulgin, A.T., *J. Chromatogr.*, 1967, **30**, 54 (*isol, synth*)

1,5,9,10-Tetramethylanthracene T-80137

[120231-35-8]

$C_{18}H_{18}$ M 234.340
Yellow needles (MeOH). Mp 71-72°.

Meador, M.A. *et al*, *J. Org. Chem.*, 1989, **54**, 2336 (*synth, pmr, ms*)

1,8,9,10-Tetramethylanthracene T-80138

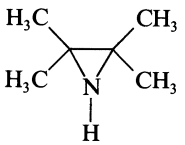
[120231-34-7]

$C_{18}H_{18}$ M 234.340
Yellow cryst. (MeOH/Et_2O). Mp 80-82°.

Meador, M.A. *et al*, *J. Org. Chem.*, 1989, **54**, 2336 (*synth, pmr, ms*)

2,2,3,3-Tetramethylaziridine T-80139

[5910-14-5]



$C_6H_{13}N$ M 99.175
Liq. Bp_{744} 104-104.5°.

1-Me: [108065-02-7]. *1,2,2,3,3-Pentamethylaziridine*
$C_7H_{15}N$ M 113.202
Obt. as salts.

1-Me; B,MeSO$_3$CF$_3$: [113181-25-2].
Cryst. (Me_2CO). Mp 176° dec.

1-Me; B,MeI: [113181-30-9].
Solid. Mp 181° dec.

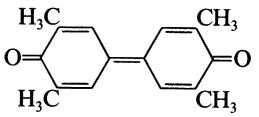
1-Me; B,MeClO$_4$: [113181-31-0].
Solid. Mp 194° dec.

Closs, G.L. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 6068 (*synth, ir, pmr*)
Lillocci, C., *J. Org. Chem.*, 1988, **53**, 1733 (*deriv, synth, pmr, ms*)

3,3′,5,5′-Tetramethyl[bi-2,5-cyclohexadien-1-ylidene]-4,4′-dione, 8CI T-80140

4-(3,5-Dimethyl-4-oxo-2,5-cyclohexadien-1-ylidene)-2,6-dimethyl-2,5-cyclohexadien-1-one, 9CI. 3,3′,5,5′-Tetramethyl-4,4′-diphenoquinone

[4906-22-3]



$C_{16}H_{16}O_2$ M 240.301
Small red needles (AcOH). Mp 208° dec.

Brown, B.R. *et al*, *J. Chem. Soc.*, 1954, 1280 (*synth, ir*)

2,2,3,3-Tetramethyl-1,4-butanediol T-80141

[10519-69-4]

$$HOCH_2C(CH_3)_2C(CH_3)_2CH_2OH$$

$C_8H_{18}O_2$ M 146.229
Fine cryst. (hexane/$CHCl_3$). Mp 209-211°.

Bis-4-methylbenzenesulfonyl: [70178-81-3].
Cryst. (hexane/$CHCl_3$). Mp 110-111°.

Sowinsky, F.A.F. *et al*, *J. Org. Chem.*, 1979, **44**, 2369 (*synth, ir, pmr, ms*)
Juaristi, E. *et al*, *J. Org. Chem.*, 1988, **53**, 3334 (*synth, pmr, ir*)

2,2,3,3-Tetramethyl-1,4-butanedithiol T-80142

[114763-99-4]

$$HSH_2CC(CH_3)_2C(CH_3)_2CH_2SH$$

$C_8H_{18}S_2$ M 178.362
Pale yellow solid.

Di-Ac: [114764-00-0].
$C_{12}H_{22}O_2S_2$ M 262.437
Slightly yellow solid. Mp 56-58°.

Jauristi, E. *et al*, *J. Org. Chem.*, 1989, **53**, 3334 (*synth, pmr*)

2,2,4,4-Tetramethyl-1,3-cyclobutanedione T-80143

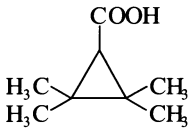
[933-52-8]

$C_8H_{12}O_2$ M 140.182
Mp 115-116°. Bp 159-161°.

Erickson, J.L.E. *et al*, *J. Am. Chem. Soc.*, 1946, **68**, 492 (*synth, props*)

2,2,3,3-Tetramethylcyclopropane-carboxylic acid, 9CI T-80144

[15641-58-4]

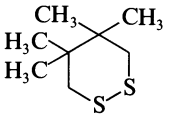


$C_8H_{14}O_2$ M 142.197
Prisms (AcOH aq.).

Meshcheryakov, A.P. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1960, 931 (*synth*)
Jones, P.G. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 1752 (*cryst struct*)

4,4,5,5-Tetramethyl-1,2-dithiane T-80145

[114763-96-1]



$C_8H_{16}S_2$ M 176.346
Solid by subl. $Bp_{0.5}$ 32° subl.

1-Oxide: [114763-95-0].
$C_8H_{16}OS_2$ M 192.346
Solid by subl. Mp 187-189°. $Bp_{0.5}$ 80-85° subl.

Juaristi, E. *et al*, *J. Org. Chem.*, 1988, **53**, 3334 (*synth, pmr, ir, cmr*)

2,2,5,5-Tetramethyl-3,4-hexanedione T-80146

*Di-*tert*-butyl diketone*

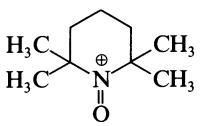
[4388-88-9]

$(H_3C)_3CCOCOC(CH_3)_3$

$C_{10}H_{18}O_2$ M 170.251
Yellow liq.

Backer, H.J., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1938, **57**, 967 (*synth*)
Griesbaum, K. *et al*, *Chem. Ber.*, 1988, **121**, 1795 (*synth, ir, pmr*)

2,2,6,6-Tetramethyl-1-oxopiperidinium (1+) T-80147



$C_9H_{18}NO^{\oplus}$ M 156.247 (ion)

Chloride: [26864-01-7].
$C_9H_{18}ClNO$ M 191.700
Oxidising agent. Buff solid. Mp 118-119°. Moisture and light sensitive.

Golubev, V.A. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, (*Engl. trans.*), 1970, 186 (*synth, uv, ir*)
Hunter, D.H. *et al*, *Tetrahedron Lett.*, 1984, **25**, 603 (*use*)
Hunter, D.H. *et al*, *J. Org. Chem.*, 1988, **53**, 1278 (*synth, bibl*)

2,2,4,4-Tetramethyl-3-pentanol, 9CI T-80148

*Di-*tert*-butylcarbinol*

[14609-79-1]

$(H_3C)_3CCH(OH)C(CH_3)_3$

$C_9H_{20}O$ M 144.256
Cryst. Mp 50°.

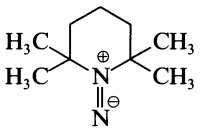
Phenylurethane: Mp 121-122°.

Bartlett, P.D. *et al*, *J. Am. Chem. Soc.*, 1945, **67**, 141 (*synth*)
Patterson, L.K. *et al*, *J. Phys. Chem.*, 1966, **70**, 3745 (*pmr*)
Roberts, D.D. *et al*, *J. Org. Chem.*, 1988, **53**, 2573 (*synth*)

N-(2,2,6,6-Tetramethylpiperidyl)nitrene T-80149

*1-(Imino-*N*)-2,2,6,6-tetramethylpiperidinium hydroxide inner salt, 9CI*

[76372-13-9]



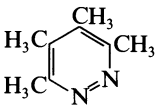
$C_9H_{18}N_2$ M 154.255
Stable deriv. of isodiazene $H_2N^{\oplus}{=}N^{\ominus}$. Reg. no. refers to ^{15}N-labelled compd. Intense purple soln. at −78°.

[76372-12-8]

Hinsberg, W.D. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 1608 (*synth, uv*)

3,4,5,6-Tetramethylpyridazine T-80150

[22868-72-0]

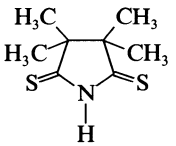


$C_8H_{12}N_2$ M 136.196
Mp 65-67° (69° dec.).

Maier, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1971, **10**, 809 (*synth, pmr*)
Shepherd, M.K., *J. Chem. Soc., Perkin Trans.* 1, 1988, 961 (*synth*)

3,3,4,4-Tetramethyl-2,5-pyrrolidinedithione T-80151

2,2,3,3-Tetramethyldithiosuccinimide

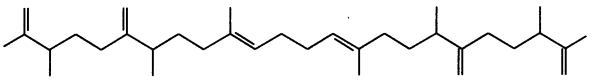


$C_8H_{13}NS_2$ M 187.329
Yellow prisms (Et_2O/pentane). Mp 92.5-94.5°.

Battersby, A.R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 1577 (*synth, ir, pmr, ms*)

Tetramethylsqualene T-80152

2,3,7,10,15,18,22,23-Octamethyl-7,19-dimethylene-1,10,14,23-tetracosatetraene



$C_{34}H_{58}$ M 466.832
Constit. of *Botryococcus braunii* var. *showa*. Oil. $[\alpha]_D^{25}$ +6° (c, 0.21 in $CHCl_3$).

Huang, Z. *et al*, *Phytochemistry*, 1989, **28**, 1467.

1,1,4,4-Tetramethyl-2-tetrazene, 9CI T-80153

Bis(dimethylamino)diazene

[6130-87-6]

$Me_2NN{=}NNMe_2$

$C_4H_{12}N_4$ M 116.166
Yellow oil. Bp 130°, Bp_{15} 32°.

▷ Explodes on heating above b.p.

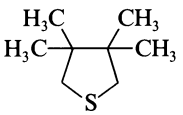
Picrate: Cryst. Mp 80° dec.

[39247-67-1]

Renouf, E., *Chem. Ber.*, 1880, **13**, 2169 (*synth, haz*)
McBride, W.R. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 572 (*synth, uv*)
Bull, W.E. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 2516 (*synth, uv*)
Good, A. *et al*, *J. Chem. Soc. B*, 1967, 684 (*props*)
Harris, W.C. *et al*, *Inorg. Chem.*, 1974, **13**, 2297 (*struct, ir*)
Mason, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 2522 (*N- nmr*)
Heymanns, P. *et al*, *Tetrahedron*, 1986, **42**, 2511 (*props*)

3,3,4,4-Tetramethylthiolane T-80154

[114763-97-2]



$C_8H_{16}S$ M 144.280
Solid. $Bp_{0.5}$ 40.4°.

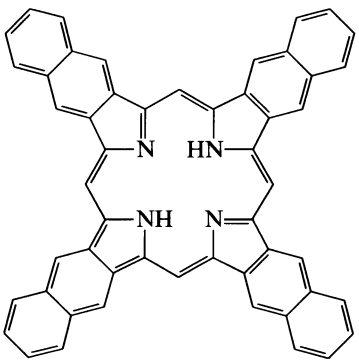
1-Oxide: [114763-98-3].
$C_8H_{16}OS$ M 160.280
Cryst. V. hygroscopic, no Mp could be obt.

Juaristi, E. *et al*, *J. Org. Chem.*, 1988, **53**, 3338 (*synth, pmr, ir, ms*)

37*H*,39*H*-Tetranaphtho-[2,3-*b*:2′,3′-*g*:2″,3″-*l*:2‴-3‴-*q*]porphine, 9CI T-80155

Tetra(2,3-naphtho)porphin

[73523-25-8]

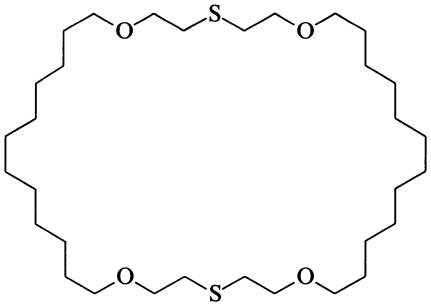


$C_{52}H_{30}N_4$ M 710.836
Green powder. Various complexes prepd.

Rein, M. *et al*, *Chem. Ber.*, 1988, **121**, 1601 (*synth, ir, uv*)

1,7,20,26-Tetraoxa-4,23-dithiacycloctatriacontane, 9CI T-80156

[116186-12-0]



$C_{32}H_{64}O_4S_2$ M 576.987
S-Oxidised or methylated derivs are bipolar, water insoluble amphiphiles. Platelets (2-propanol). Mp 69°.

B, 2MeClO$_4$: Powder (MeOH). Mp 95°.

S,S′-Dioxide: [116186-15-3].
$C_{32}H_{64}O_6S_2$ M 608.986
Cryst. (EtOH). Mp 72°.

S,S′-Tetroxide: [116186-14-2].
$C_{32}H_{64}O_8S_2$ M 640.985
Platelets (EtOH). Mp 75°.

Fuhrhop, J.-H. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6840 (*synth, derivs, use, ir, ms, pmr*)

Tetraphenoxyethene T-80157

1,1′,1″,1‴-[1,2-Ethenediylidenetetrakis(oxy)]tetrakisbenzene, 9CI. Tetraphenoxyethylene

[4895-47-0]

$(PhO)_2C{=}C(OPh)_2$

$C_{26}H_{20}O_4$ M 396.442
Cryst. (pet. ether). Mp 170°.

McDonald, R.N. *et al*, *J. Org. Chem.*, 1965, **30**, 4372 (*synth*)
Scheeren, J.W. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1973, **92**, 11 (*synth*)

1,1,5,5-Tetraphenyl-1,4-pentadien-3-one T-80158

[21086-26-0]

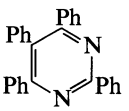
$Ph_2C{=}CHCOCH{=}CPh_2$

$C_{29}H_{22}O$ M 386.492
Yellow cryst. (EtOH aq.). Mp 155°.

Marin, G. *et al*, *Bull. Soc. Chim. Fr.*, 1958, 1594 (*synth*)

Tetraphenylpyrimidine T-80159

[14277-91-9]

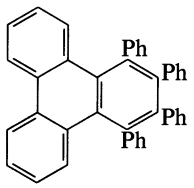


$C_{28}H_{20}N_2$ M 384.479
Cryst. (EtOH). Mp 185-187°.

Garcia Martinéz, A. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1237 (*synth, cmr*)

1,2,3,4-Tetraphenytriphenylene T-80160

[36262-81-4]



$C_{42}H_{28}$ M 532.683
Shows twisted polycyclic nucleus. Cryst. (CH_2Cl_2/Me_2CO). Mp 292-293°, Mp >350°.

Dilthey, W. *et al*, *Ber.*, 1938, **71**, 974 (*synth*)
Pascal, R.A. *et al*, *J. Org. Chem.*, 1988, **53**, 1687 (*synth, pmr, cryst struct*)

1-Tetratriacontanol, 9CI T-80161

Sapiol

[28484-70-0]

$H_3C(CH_2)_{32}CH_2OH$

$C_{34}H_{70}O$ M 494.926
Isol. from candelilla, cotton waxes and leaves of *Sapium indicum*. Mp 92°.

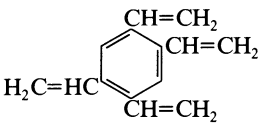
[103215-66-3]

Chibnall, A.C. *et al*, *Biochem. J.*, 1934, **28**, 2189 (*isol*)
Mazliak, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1960, **251**, 2393 (*isol*)
Japan. Pat., 80 129 292, (1980); *ca*, **94**, 120844r (*synth*)

1,2,4,5-Tetravinylbenzene T-80162

1,2,4,5-Tetraethenylbenzene, 9CI

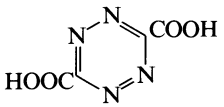
[117382-80-6]



$C_{14}H_{14}$ M 182.265
Solid. Mp 30-31°. $Bp_{0.001}$ 80-90° (Kugelrohr).

Schrievers, T. *et al*, *Synthesis*, 1988, 330 (*synth, ir, pmr, cmr, ms*)

1,2,4,5-Tetrazine-3,6-dicarboxylic acid T-80163



$C_4H_2N_4O_4$ M 170.084

Di-Na salt: [113631-48-4].
Red powder.

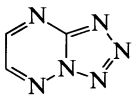
Di-Me ester: [2166-14-5].
$C_6H_6N_4O_4$ M 198.138
Bright red cryst. solid. Mp 173-175°.

Dinitrile: [16453-19-3]. *3,6-Dicyano-1,2,4,5-tetrazine*
C_4N_6 M 132.084
Forms charge-transfer complexes. Orange cryst. by subl. Mp 91°.

Curtius, T. *et al*, *Ber.*, 1907, **40**, 84 (*synth*)
Mason, S.F., *J. Chem. Soc.*, 1959, 1247 (*uv*)
Weininger, S.J. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2050 (*dinitrile*)
Boger, D.L. *et al*, *J. Org. Chem.*, 1985, **50**, 5377 (*synth, pmr, ir, uv*)
Beilin, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 1579 (*dinitrile*)

Tetrazolo[1,5-*b*][1,2,4]triazine T-80164

[32484-95-0]



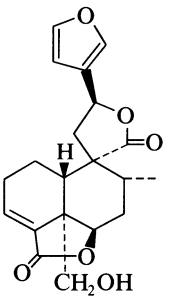
$C_3H_2N_6$ M 122.089
Cryst. (MeOH). Mp 174-176°.

Goodman, M.M. *et al*, *J. Org. Chem.*, 1976, **41**, 2860 (*synth, pmr, cryst struct, ir*)
Willer, R.L., *J. Org. Chem.*, 1988, **53**, 5371 (*synth*)

Teuscorodonin T-80165

Updated Entry replacing T-20155
Teuscordonin

[87376-66-7]

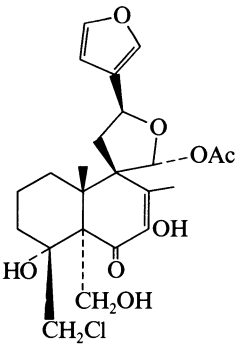


$C_{20}H_{22}O_6$ M 358.390
Constit. of *Teucrium scorodonia*. Cryst. (EtOAc/hexane). Mp 189-191°. $[\alpha]_D^{22}$ +110.8° (c, 0.204 in $CHCl_3$).

12-Epimer: 12-Epiteuscordonin. 12-Epiteuscorodonin
$C_{20}H_{22}O_6$ M 358.390
Constit. of *T. bicolor*. Cryst. (EtOAc/pet. ether). Mp 199-203°.

Marco, J.L. *et al*, *Phytochemistry*, 1983, **22**, 727.
Labbe, C. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 871 (*epimer*)

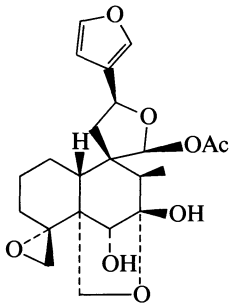
Teuvincentin A T-80166



$C_{24}H_{29}ClO_9$ M 496.940
Constit. of *Teucrium polium*. Cryst. (EtOAc/hexane). Mp 200-201° dec. $[\alpha]_D^{20}$ −92.7° (c, 0.192 in $CHCl_3$).

Carreiras, M.C. *et al*, *Phytochemistry*, 1989, **28**, 1453 (*isol, cryst struct*)

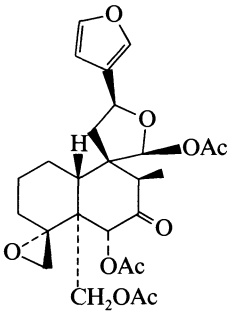
Teuvincentin B T-80167



$C_{22}H_{28}O_8$ M 420.458
Constit. of *Teucrium polium*. Cryst. (EtOAc/hexane). Mp 194-197°. $[\alpha]_D^{20}$ −27.1° (c, 0.17 in $CHCl_3$).

Carreiras, M.C. *et al*, *Phytochemistry*, 1989, **28**, 1453 (*isol, cryst struct*)

Teuvincentin C T-80168

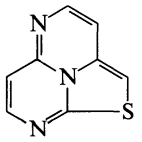


$C_{26}H_{32}O_{10}$ M 504.533
Constit. of *Teucrium polium*. Cryst. (EtOAc). Mp 220-225°. $[\alpha]_D^{22}$ −8.1° (c, 0.246 in $CHCl_3$).

Carreiras, M.C. *et al*, *Phytochemistry*, 1989, **28**, 1453.

1-Thia-5,8,8*b*-triazaacenaphthylene T-80169

[70304-49-3]



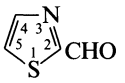
$C_8H_5N_3S$ M 175.214
Maroon cryst. (1-chlorobutane). Mp 117-119° dec.

Selby, T.P., *J. Org. Chem.*, 1988, **53**, 2386 (*synth, ir, pmr*)

2-Thiazolecarboxaldehyde T-80170

2-Formylthiazole

[10200-59-6]



C_4H_3NOS M 113.140
Liq. Bp_{11} 61-63°, Bp_3 36-37°.

Oxime: [13838-77-2].
$C_4H_4N_2OS$ M 128.154
Mp 118-120°.

Phenylhydrazone: Cryst. (EtOH aq.). Mp 117-118°.

2,4-Dinitrophenylhydrazone: Cryst. (EtOH). Mp 241-243°.

Thiosemicarbazone: Yellowish cryst. Mp 198°.

Di-Et acetal: 2-(Diethoxymethyl)thiazole
$C_8H_{13}NO_2S$ M 187.262
Bp_9 103-104°.

Beyer, H. *et al*, *Chem. Ber.*, 1957, **90**, 2372 (*synth*)
Iversen, P.E. *et al*, *Acta Chem. Scand.*, 1966, **20**, 2649 (*synth*)
Dondoni, A. *et al*, *Synthesis*, 1987, 998 (*synth, ir, pmr*)

4-Thiazolecarboxaldehyde T-80171

4-Formylthiazole

[3364-80-5]

C_4H_3NOS M 113.140
Prisms (hexane). Mp 65-66°. Bp_{14} 99-104°.

Oxime: [41827-98-9].
$C_4H_4N_2OS$ M 128.154
Mp 185-186°.

2,4-Dinitrophenylhydrazone: Orange-red needles (MeOH). Mp 250-252°.

Erne, M. *et al*, *Helv. Chim. Acta*, 1951, **34**, 143 (*synth*)
Campaigne, E. *et al*, *J. Med. Chem.*, 1959, **1**, 577 (*synth*)
Dondoni, A. *et al*, *Synthesis*, 1987, 998 (*synth, pmr, ms*)

5-Thiazolecarboxaldehyde T-80172

5-Formylthiazole

[1003-32-3]

C_4H_3NOS M 113.140
Oil. Bp_{16} 92-94°.

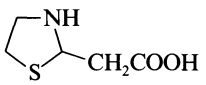
Oxime: [116045-57-9].
$C_4H_4N_2OS$ M 128.154
Mp 197-198°.

2,4-Dinitrophenylhydrazone: Red cryst. (MeOH). Mp 238-240°.

Semicarbazone: Plates (MeOH). Mp 210-212°.

Erne, M. *et al*, *Helv. Chim. Acta*, 1951, **34**, 143 (*synth*)
Dondoni, A. *et al*, *Synthesis*, 1987, 998 (*synth, pmr, ms*)

2-Thiazolidineacetic acid, 9CI T-80173



$C_5H_9NO_2S$ M 147.198
β-Lactam intermediate.

(±)-*form*

B,HCl: [98316-98-4].
Needles (EtOH/Et_2O). Mp 103-105°.

tert-*Butyl ester:* [98317-14-7].
$C_9H_{17}NO_2S$ M 203.305
Oil.

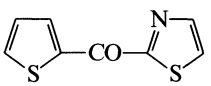
[98316-97-3]

Chiba, T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 1845 (*synth, ir, pmr*)

2-Thiazolyl 2-thienyl ketone T-80174

2-Thiazolyl-2-thienylmethanone, 9CI

[104542-82-7]

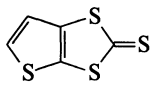


$C_8H_5NOS_2$ M 195.266
Oil.

Dondoni, A. *et al*, *J. Org. Chem.*, 1988, **53**, 1748 (*synth, ir, pmr*)

Thieno[2,3-*d*]-1,3-dithiole-2-thione T-80175

[67188-88-9]

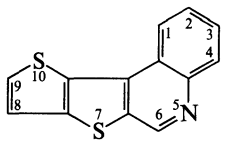


$C_5H_2S_4$ M 190.335
Red needles. Mp 125-125.5°.

Engler, E.M. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3769 (*synth, ir, pmr*)
Litvinov, V.P. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1982, 642; 1983, 1901 (*synth, ir, ms*)

Thieno[2′,3′:4,5]thieno[2,3-*c*]quinoline T-80176

[119647-21-1]

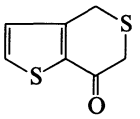


$C_{13}H_7NS_2$ M 241.337
Yellow prisms (C_6H_6). Mp 182-183°.

Castle, S.L. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1363 (*synth, pmr*)

4*H*-Thieno[3,2-*c*]thiopyran-7(6*H*)-one T-80177

[16401-39-1]



$C_7H_6OS_2$ M 170.256
Cryst. (EtOH aq.). Mp 67°. Bp_{18} 180-180.5°.

Oxime: [16470-67-0].
$C_7H_7NOS_2$ M 185.270
Needles (C_6H_6). Mp 190°.

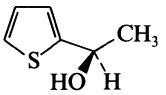
2,4-Dinitrophenylhydrazone: Red cryst. (EtOH/C_6H_6). Mp 244°.

Cagniant, P. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 2597 (*synth, pmr*)

1-(2-Thienyl)ethanol T-80178

α-Methyl-2-thiophenemethanol, 9CI. Methyl-2-thienylcarbinol. 2-(1-Hydroxyethyl)thiophene

[2309-47-9]



(*R*)-*form*

C_6H_8OS M 128.195

(***R***)-***form*** [86527-10-8]
Bp_7 87-89°. $[\alpha]_D$ +13.10° (neat).

(***S***)-***form*** [27948-39-6]
Bp_1 55°. $[\alpha]_D^{22}$ −12.65° (neat).

(±)-***form*** [115510-91-3]
Liq. Bp_{13} 98-99°. n_D^{20} 1.5420.

Phenylurethane: Plates. Mp 85° (84.2-84.9°).

[84194-85-4, 86561-31-1]

Kuhn, R. *et al*, *Justus Liebigs Ann. Chem.*, 1941, **547**, 293 (*synth*)
Weber, S. *et al*, *J. Org. Chem.*, 1962, **27**, 1258 (*synth*)
Caullet, C., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **260**, 1599 (*ir*)
Cervinka, O. *et al*, *Z. Chem.*, 1969, **9**, 448 (*synth, abs config*)
Noyce, D.S. *et al*, *J. Org. Chem.*, 1972, **37**, 2615 (*synth, pmr*)
Giumanini, A.G. *et al*, *J. Org. Chem.*, 1976, **41**, 2187 (*synth, ir, ms*)
Ziffer, H. *et al*, *J. Org. Chem.*, 1983, **48**, 3017 (*abs config*)
Chandrasekharan, J. *et al*, *J. Org. Chem.*, 1985, **50**, 5446 (*synth*)
Takeshita, M. *et al*, *Heterocycles*, 1987, **26**, 3051 (*synth, pmr*)
Brown, H.C. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1539 (*synth*)
Rosini, C. *et al*, *J. Org. Chem.*, 1988, **53**, 4579 (*pmr*)

1-(3-Thienyl)ethanol T-80179

α-Methyl-3-thiophenemethanol, 9CI. Methyl-3-thienylcarbinol. 3-(1-Hydroxyethyl)thiophene

[14861-60-0]

C_6H_8OS M 128.195

(±)-***form***
Liq. d_4^{16} 1.188. Bp_4 85°. n_D^{20} 1.5473.

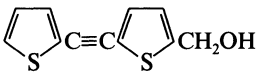
Ac:
$C_8H_{10}O_2S$ M 170.232
Liq. $Bp_{3.5}$ 87°. n_D^{20} 1.5081.

Troyanowsky, C., *Bull. Soc. Chim. Fr.*, 1955, 424 (*synth*)
Gronowitz, S. *et al*, *J. Chem. Soc.*, 1963, 3881 (*ir*)
Janda, M. *et al*, *Collect. Czech. Chem. Commun.*, 1967, **32**, 2675 (*synth*)
Macco, A.A. *et al*, *J. Org. Chem.*, 1978, **43**, 1591 (*synth*)
Abarca, B. *et al*, *Tetrahedron*, 1987, **43**, 269 (*synth*)

5-(2-Thienylethynyl)-2-thiophenemethanol, 9CI T-80180

2-Hydroxymethyl-5-(2-thienylethynyl)thiophene

[36687-74-8]

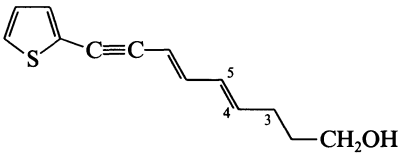


$C_{11}H_8OS_2$ M 220.316
Constit. of the roots of *Berkheya* and *Cuspida* spp. Oil.

Ac: [36687-73-7].
$C_{13}H_{10}O_2S_2$ M 262.353
Constit. of *B.* and *C.* spp.

Bohlmann, F. *et al*, *Chem. Ber.*, 1972, **105**, 1245; 1974, **103**, 2115 (*isol, struct, synth*)

9-(2-Thienyl)-4,6-nonadien-8-yn-1-ol, 9CI T-80181



$C_{13}H_{14}OS$ M 218.319
Isol. from roots of *Xeranthemum cylindraceum*. λ_{max} 316, 337 nm.

Ac: 1-Acetoxy-9-(2-thienyl)-4,6-nonadien-8-yne
$C_{15}H_{16}O_2S$ M 260.356
Isol. from *X. cylindraceum*. Cryst. (pet. ether). Mp 32°.

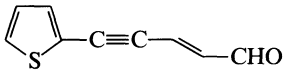
Deoxy, 3-hydroxy: ***9-(2-Thienyl)-4,6-nonadien-8-yn-3-ol, 9CI***
$C_{13}H_{14}OS$ M 218.319
Isol. from roots of *Anthemis saguramica*. Oil. λ_{max} 317, 338.5 nm (ε 26, 700; 21, 700).

Deoxy, 3-hydroxy, 4,5-dihydro: ***9-(2-Thienyl)-6-nonen-8-yn-3-ol, 9CI***
$C_{13}H_{16}OS$ M 220.335
Isol. from *A. saguramica*. Oil. λ_{max} 277sh, 292, 308.5 nm (ε 14,600; 19,700; 16,200).

Deoxy, 3-acetoxy, 4,5-dihydro: [14686-18-1].
$C_{14}H_{18}O_2S$ M 250.361
Isol. from *Matricaria* sp. Oil. λ_{max} 309, 292 nm.

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 2125; 1966, **99**, 1642; 1967, **100**, 611 (*isol, struct, uv, ir, pmr, derivs*)
Bohlmann, F. *et al*, *Tetrahedron Lett.*, 1965, 1385 (*synth*)

5-(2-Thienyl)-2-penten-4-ynal, 9CI T-80182

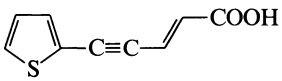


C_9H_6OS M 162.212

(E)-form [62826-56-6]
Isol. from roots of *Anthemis saguramica*. Yellow cryst. (pet. ether). Mp 41.5°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1966, **99**, 1642 (*isol, uv, ir, pmr, struct, synth*)

5-(2-Thienyl)-2-penten-4-ynoic acid T-80183



$C_9H_6O_2S$ M 178.211

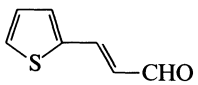
(E)-form
Me ester:
$C_{10}H_8O_2S$ M 192.238
Isol. from above ground parts of *Anthemis fuscata*. Cryst. (pet. ether). Mp 67°.

(Z)-form
Me ester: Oil.

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 1733; 1965, **98**, 1411 (*isol, uv, struct, synth*)

3-(2-Thienyl)-2-propenal, 9CI T-80184

3-(2-Thienyl)acrolein
[14756-03-7]



C_7H_6OS M 138.190

(E)-form [39511-07-4]
Yellowish oil. $Bp_{0.4}$ 105-108°, $Bp_{0.15}$ 88-95°.
Semicarbazone: Mp 218-219°.

Keskin, H. *et al*, *J. Org. Chem.*, 1951, **16**, 199 (*synth, deriv*)
Savin, F.I. *et al*, *Khim. Geterotsikl. Soedin.*, 1972, 1331 (*conformn*)
Kossmehl, G. *et al*, *Chem. Ber.*, 1974, **107**, 2791 (*synth*)

3-(3-Thienyl)-2-propenal, 9CI T-80185

3-(3-Thienyl)acrolein
[72078-30-9]
C_7H_6OS M 138.190

(E)-form
Oil. Bp_5 125-128°.

Klemm, L.H. *et al*, *J. Heterocycl. Chem.*, 1965, **2**, 225 (*synth*)

2,3′-Thiobispyridine T-80186

2-(3-Pyridinylthio)pyridine, 9CI. 2-Pyridyl 3-pyridyl sulfide
[72890-91-6]
$C_{10}H_8N_2S$ M 188.253
Oil.
Picrate: Cryst. (H_2O). Mp 174-175°.

Krowicki, K., *Pol. J. Chem.* (*Rocz. Chem.*), 1978, **52**, 2349 (*synth*)
Summers, L.A., *J. Heterocycl. Chem.*, 1987, **24**, 533 (*rev*)

2,4′-Thiobispyridine T-80187

2-(4-Pyridinylthio)pyridine, 9CI. 2-Pyridyl 4-pyridyl sulfide
[76093-03-3]
$C_{10}H_8N_2S$ M 188.253
Derivatives have bactericidal, fungicidal and herbicidal properties. Oil.
Picrate: Mp 167-168°.

Boduszek, B. *et al*, *Monatsh. Chem.*, 1980, **111**, 1111 (*synth, pmr*)
Summers, L.A., *J. Heterocycl. Chem.*, 1987, **24**, 533 (*rev*)

3,4′-Thiobispyridine T-80188

3-(4-Pyridinylthio)pyridine, 9CI. 3-Pyridyl 4-pyridyl sulfide
[72890-90-5]
$C_{10}H_8N_2S$ M 188.253
Oil.
Dipicrate: Cryst. (H_2O). Mp 190-192°.

Krowicki, K., *Pol. J. Chem.* (*Rocz. Chem.*), 1978, **52**, 2349 (*synth*)
Summers, L.A., *J. Heterocycl. Chem.*, 1987, **24**, 533 (*rev*)

3-Thiocyanato-1-propene T-80189

Allyl thiocyanate. Allylrhodamide. Thiocyanic acid 2-propenyl ester, 9CI
[764-49-8]

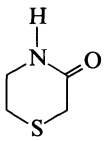
$$H_2C{=}CHCH_2SCN$$

C_4H_5NS M 99.156
Present in seeds of *Brassica juncea*. Prod. from Sinigrin by enzymes in *Thlaspi arvense*. Pungent oil. d^{15} 1.056. Bp 161°. Rearr. on standing.

Gmelin, R. *et al*, *Acta Chem. Scand.*, 1959, **13**, 1474.
Kirk, L.D. *et al*, *J. Am. Oil Chem. Soc.*; 1964, **41**, 599.
Emerson, D.W., *J. Chem. Educ.*, 1971, **48**, 81 (*synth*)

3-Thiomorpholinone, 9CI T-80190

[20196-21-8]



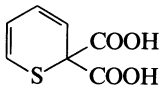
C_4H_7NOS M 117.171
Long needles (EtOAc), cryst. (CH_2Cl_2/Et_2O). Mp 92-93°. Bp_{18} 185°.

S-Oxide:
$C_4H_7NO_2S$ M 133.171
Mp 141-143°.

S-Dioxide:
$C_4H_7NO_3S$ M 149.170
Mp 171-173°.

Bestian, H., *Justus Liebigs Ann. Chem.*, 1950, **566**, 242 (*synth*)
Hall, H.K., *J. Am. Chem. Soc.*, 1958, **80**, 6404 (*synth, use*)
Lehr, H. *et al*, *J. Med. Chem.*, 1963, **6**, 136 (*synth, derivs*)
De Filippo, D. *et al*, *Gazz. Chim. Ital.*, 1968, **98**, 64 (*synth*)
Nagarajan, K. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 720 (*synth, ir, use*)
Matarese, R.M. *et al*, *J. Chromatogr.*, 1984, **294**, 413 (*tlc, ms*)
Ramasubbu, N. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 2016 (*cryst struct*)

2*H*-Thiopyran-2,2-dicarboxylic acid T-80191



$C_7H_6O_4S$ M 186.188

Di-Me ester: [117699-51-1].
$C_9H_{10}O_4S$ M 214.242
Yellow oil.

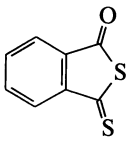
*Di-*tert*-butyl ester:* [102203-47-4].
$C_{15}H_{22}O_4S$ M 298.402
Cryst. (MeOH). Mp 93-94°.

Bowles, T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 803 (*synth, ir, pmr*)

3-Thioxo-1(3*H*)-benzo[*c*]thiophenone T-80192

Phthalic thiothionoanhydride

[112270-93-6]



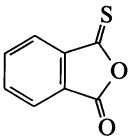
$C_8H_4OS_2$ M 180.251
Black needles (hexane). Mp 87-88°.

Raasch, M.S. *et al*, *J. Org. Chem.*, 1988, **53**, 891 (*synth, ir, uv, ms, pmr*)

3-Thioxo-1(3*H*)-isobenzofuranone, 9CI T-80193

Thionophthalic anhydride

[13699-68-8]



$C_8H_4O_2S$ M 164.184
Red cryst. by subl. Mp 91-96° dec. Readily isom.

Shants, C.M. *et al*, *J. Org. Chem.*, 1967, **32**, 3709 (*synth, uv*)

3-Thujene T-80194

2-Methyl-5-(1-methylethyl)bicyclo[3.1.0.]hex-2-ene, 9CI. 5-Isopropyl-2-methylbicyclo[3.1.0]hex-2-ene. α-Thujene. Origanene

[2867-05-2]

$C_{10}H_{16}$ M 136.236
Isol. from *Boswellia serrata*, *Eucalyptus* spp., *Thuja* spp. and many other plant oils. Liq. Bp 151-153°. $[\alpha]_D$ +38.84°.

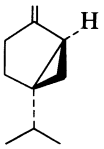
Norin, T., *Acta Chem. Scand.*, 1962, **16**, 640 (*abs config*)
Thomas, A.F. *et al*, *Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Wrolstad, R.E. *et al*, *J. Agric. Food Chem.*, 1964, **12**, 501 (*ir*)
Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985, no. 59 (*occur*)

4(10)-Thujene T-80195

Updated Entry replacing T-02142

4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane, 9CI. 1-Isopropyl-4-methylenebicyclo[3.1.0]hexane. ***Sabinene***

[3387-41-5]



(+)-*form*

$C_{10}H_{16}$ M 136.236

(+)-***form*** [2009-00-9]
Constit. of various essential oils, e.g. *Juniperus sabina*, *Myristica fragrans*. Bp_{160} 163-165°. $[\alpha]_D$ +95° (c, 20 in CCl_4).

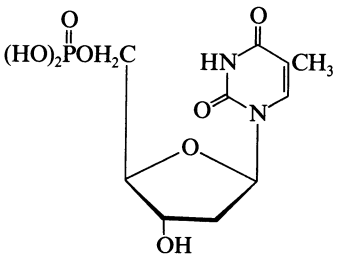
(−)-***form*** [10408-16-9]
Constit. of *Laurus nobilis*, *Pinus muricata* and some other plants. Liq. Bp 162-166°. $[\alpha]_D$ −89°.

Jaureguiberry, G. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 1985 (*isol, ir, pmr*)
Ryhage, R. *et al*, *Acta Chem. Scand.*, 1963, **17**, 2025 (*ms*)
Banthorpe, D.V. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 177 (*biosynth*)
Fanta, W.I. *et al*, *J. Org. Chem.*, 1968, **33**, 1656 (*synth*)
Acharya, S.P. *et al*, *J. Org. Chem.*, 1969, **34**, 3015 (*abs config*)
Whitaker, D. *et al*, *Chem. Rev.*, 1972, **72**, 305 (*rev*)
Karrer, W. *et al*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd Ed., Birkhäuser Verlag, Basel, 1972-1985, no. 60 (*occur*)

Thymidine 5′-phosphate T-80196

Thymidine 5′-(dihydrogen phosphate), 10CI. 5′-Thymidylic acid, 9CI

[365-07-1]



$C_{10}H_{15}N_2O_8P$ M 322.211
Occurs in tRNA, human lymphocytes, brain and liver. pK_{a1} 6.36, pK_{a2} 9.90.

Di-Na salt: Dihydrate. Mp >300°.

Ba salt: $[\alpha]_D^{17}$ −3.0° (*c*, 2 in H_2O).

Dibrucine salt: Needles (EtOH aq.). Mp 175°.

Dibenzyl ester:
$C_{24}H_{27}N_2O_8P$ M 502.460
Foam ($CHCl_3$/cyclohexane).

[33430-62-5]

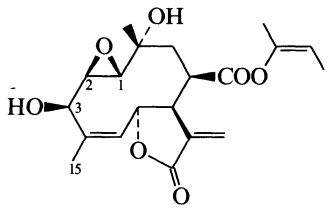
Sprecher, C.A. *et al*, *Biopolymers*, 1977, **16**, 2243 (*cd*)
Sagi, J.T. *et al*, *Nucleic Acids Res.*, 1977, **4**, 2767 (*synth*)
George, A.L. *et al*, *Can. J. Chem.*, 1978, **56**, 1170 (*pmr, conformn*)
Niemezura, W.P. *et al*, *Can. J. Chem.*, 1980, **58**, 472 (*cmr, conformn*)
Samanta, S.T. *et al*, *Appl. Spectrosc.*, 1982, **36**, 306 (*raman*)
Stawinski, J., *Bull. Pol. Acad. Sci., Chem.*, 1983, **31**, 17 (*synth*)

Cadet, J. *et al*, *J. Chromatogr.*, 1983, **259**, 111 (*tlc*)
Sekine, M. *et al*, *Tetrahedron Lett.*, 1983, **24**, 5741 (*deriv*)
Sato, T., *Acta Crystallogr., Sect. C*, 1984, **40**, 736 (*cryst struct*)
Cerny, R.L. *et al*, *Anal. Biochem.*, 1986, **156**, 424 (*ms*)
Horn, T. *et al*, *Tetrahedron Lett.*, 1986, **27**, 4705 (*synth, hplc, nmr, tlc*)
Massoud, S.S. *et al*, *Inorg. Chem.*, 1988, **27**, 1447 (*props*)

Tifruticin T-80197

Updated Entry replacing T-70199

[56377-69-6]



$C_{20}H_{26}O_7$ M 378.421
Constit. of *Tithonia fruticosa*. Cryst. (EtOAc). Mp 141°. $[\alpha]_D^{22}$ −22° (c, 1.1 in $CHCl_3$).

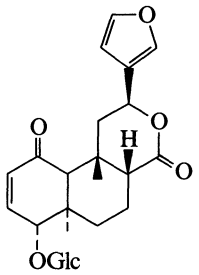
Deepoxy, 1,2-didehydro: [56377-63-0]. ***Deoxytifruticin***
$C_{20}H_{26}O_6$ M 362.422
Minor constit. of *T. fruticosa*.

3-Ketone, 15-hydroxy: [119889-30-4]. ***15-Hydroxy-3-dehydrotifruticin***
$C_{20}H_{24}O_8$ M 392.405
Constit. of *T. pedicunculata*. Pale yellow oil.

Herz, W. *et al*, *J. Org. Chem.*, 1975, **40**, 3118 (*isol*)
Baruah, N.C. *et al*, *J. Org. Chem.*, 1979, **44**, 1831 (*config*)
Pérez, A.L. *et al*, *Phytochemistry*, 1988, **27**, 3897 (*isol, deriv*)

Tinosporaside T-80198

[120163-16-8]

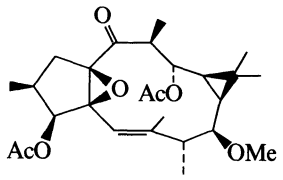


$C_{25}H_{32}O_{10}$ M 492.522
Constit. of *Tinospora cordifolia*. Needles (MeOH aq.). Mp 228-229°. $[\alpha]_D$ +65° (c, 1 in MeOH).

Khan, M.A. *et al*, *Phytochemistry*, 1989, **28**, 273.

Tirucalicine T-80199

[77573-15-0]



$C_{27}H_{38}O_9$ M 506.592
Constit. of *Euphorbia tirucalli*. Needles (EtOH). Mp 148-150°. $[\alpha]_D$ +16.13° (c, 3.41 in $CHCl_3$).

Khan, A.Q. *et al*, *Heterocycles*, 1988, **27**, 2851.

β-Tocopherol T-80200

Updated Entry replacing T-20180

3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol, 9CI. 2,5,8-Trimethyl-2-(4,8,12-trimethyltridecyl)chroman-6-ol, 8CI. 5,8-Dimethyltocol. Cumotocopherol. Neotocopherol. p-*Xylotocopherol*

[148-03-8]

$C_{28}H_{48}O_3$ M 432.685
Isol. from vegetable sources, e.g. spinach chloroplasts (*Spinacea oleracea*), soybean oil, corn oil. Antioxidant. Pale-yellow viscous oil. $Bp_{0.1}$ 200-210°. $[\alpha]_{546}^{25}$ +2.9° (EtOH). Thermostable; resistant to acids and alkalis.

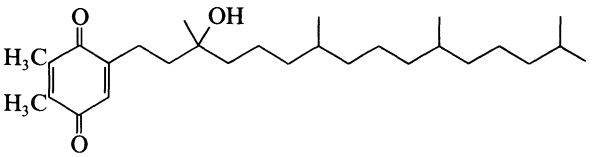
3,5-Dinitrobenzoyl: Mp 86-87°.

Ac: Pale-yellow oil. $Bp_{0.3}$ 215-220°.

[16662-70-7, 16698-35-4]

Karrer, P. *et al*, *Helv. Chim. Acta*, 1938, **21**, 1234; 1939, **22**, 260 (*synth, struct*)
Mayer, H. *et al*, *Helv. Chim. Acta*, 1963, **46**, 963 (*abs config*)
Pearson, C.K. *et al*, *Br. J. Nutr.*, 1970, **24**, 581 (*metab*)
Nakamura, A. *et al*, *Chem. Pharm. Bull.*, 1971, **19**, 2318 (*synth*)
Scheppele, S.E. *et al*, *Lipids*, 1972, **7**, 297 (*ms*)
Matsuo, M. *et al*, *Tetrahedron*, 1976, **32**, 229 (*cmr*)
Tangney, C.C. *et al*, *J. Chromatogr.*, 1979, **172**, 513 (*purifn*)
Burton, G.W. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 6472 (*props*)
Pure Appl. Chem., 1982, **54**, 1507 (*nomencl*)
Urano, S. *et al*, *Heterocycles*, 1985, **23**, 2793 (*synth*)

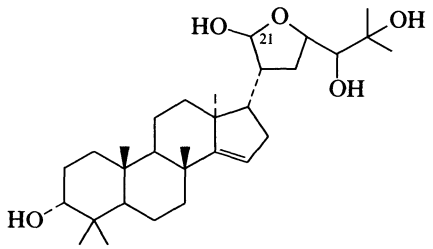
γ-Tocopheryl quinone T-80201



$C_{28}H_{48}O_3$ M 432.685
Isol. from vegetable sources, e.g. spinach chloroplasts (*Spinacea oleracea*). Oil. λ_{max} 258 nm.

Henninger, M.D. *et al*, *Biochemistry*, 1963, **2**, 1168.

Toosendanpentol T-80202

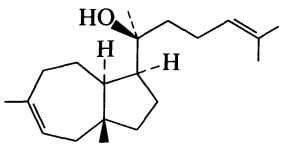


$C_{30}H_{50}O_6$ M 506.721
21-Me ether: 21-O-Methyltoosendanpentol
$C_{31}H_{52}O_6$ M 520.748
Constit. of *Melia toosendan*. Needles (Me_2CO/hexane). Mp 106-108°. $[\alpha]_D$ −52.1° (c, 0.36 in MeOH).

Inada, A. *et al*, *Heterocycles*, 1989, **28**, 383.

Tormesol T-80203

[120278-23-1]

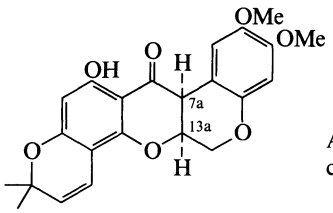


$C_{20}H_{34}O$ M 290.488
Constit. of *Halimium viscosum*. Cryst. (hexane). Mp 60-61°. $[\alpha]_D^{22}$ +30.8° (c, 1.1 in $CHCl_3$).

Urones, J.G. *et al*, *Phytochemistry*, 1989, **28**, 183.

α-Toxicarol T-80204

Updated Entry replacing T-02281
13,13a-Dihydro-6-hydroxy-9,10-dimethoxy-3,3-dimethyl-3H-bis[1]benzopyrano[3,4-b:6′,5′-e]pyran-7(7aH)-one, 9CI. Toxicarol
[82-09-7]



Absolute configuration

$C_{23}H_{22}O_7$ M 410.423
Obt. from *Derris malaccensis*. Occurs in *Crotalaria burhia* also *D. elliptica*, *Tephrosia odorata* and *T. toxicaria*. Fish poison closely related in props. to Rotenone. Greenish-yellow plates or needles (EtOAc/EtOH). Mp 125-127° (101-102°). $[\alpha]_D^{20}$ −66° (C_6H_6), $[\alpha]_D$ +58° (Me_2CO).

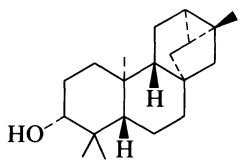
7a,*13a-Didehydro:* [59086-93-0]. ***Dehydrotoxicarol***
$C_{23}H_{20}O_7$ M 408.407
Isol. from *Amorpha fruticosa* and *D. elliptica*. Cryst. ($CHCl_3$/MeOH). Mp 263-267°.

(±)-***form***
Mp 219-223° (101-102°).

Cahn, R.S. *et al*, *J. Chem. Soc.*, 1938, 513, 734 (*isol*, *struct*)
Harper, S.H., *J. Chem. Soc.*, 1939, 812 (*isol*)
Crombie, L. *et al*, *J. Chem. Soc.*, 1962, 775 (*pmr*)
Carlson, D.G. *et al*, *Tetrahedron*, 1973, **29**, 2731 (*pmr*)
Crombie, L. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1975, 1497 (*cmr*)
Reisch, J. *et al*, *Phytochemistry*, 1976, **15**, 234 (*Dehydrotoxicarol*)

ent-3β-Trachylobanol T-80205

[120062-66-0]



$C_{20}H_{32}O$ M 288.472
Constit. of *Xylopia aromatica*.

Moraes, M.P.L. *et al*, *Phytochemistry*, 1988, **27**, 3205.

Triacontanal, 9CI T-80206

[22725-63-9]

$H_3C(CH_2)_{28}CHO$

$C_{30}H_{60}O$ M 436.803
Isol. from berries of *Vitis vinifera*, from *Brassica oleracea* leaves and from apple cuticle wax.

Radler, F. *et al*, *Aust. J. Chem.*, 1965, **18**, 1059.
Schmid, H.H.O. *et al*, *Hoppe Seyler's Z. Physiol. Chem.*, 1969, **350**, 462 (*isol*)
Japan. Pat., 59 95 236, (1982); *CA*, **101**, 170706f (*synth*)

21-Triacontenoic acid T-80207

Lumequesic acid
[67329-09-3]

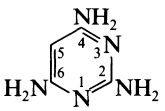
$H_3C(CH_2)_7CH{=}CH(CH_2)_{19}COOH$

$C_{30}H_{58}O_2$ M 450.787
Isol. from seed oil of *Ximenia americana*. Struct. proof not convincing from the abstr.

Boekenoogen, H.A., *Chem. Zentralbl.*, 1940, **1**, 2406.

2,4,6-Triaminopyrimidine, 8CI T-80208

2,4,6-Pyrimidinetriamine, 9CI
[1004-38-2]



$C_4H_7N_5$ M 125.133
Reagent for determination of primary aromatic amines. Prisms (EtOH). Sol. H_2O, spar. sol. EtOH, Et_2O. Mp 249-251°. pK_{a1} 6.72 (20°), pK_{a2} 1.31 (20°).

B,2HCl: Prisms.

Picrate: Needles. Mp 290°.

N^4-*Me:* [24867-24-1].
$C_5H_9N_5$ M 139.160
Yellow cryst. (EtOH). Mp 192-194°. pK_{a1} 7.21 (20°), pK_{a2} 1.05 (20°).

N^4-*Me*, N^1-*oxide:* [55973-02-9].
$C_5H_9N_5O$ M 155.159
Cryst. (MeOH/MeCN). Mp 188° dec.

N^4-*Et:* [91502-44-2].
$C_6H_{11}N_5$ M 153.186
Cryst. (CH_2Cl_2/Me_2CO). Mp 155-156°. pK_a 7.20.

N^2,N^2-*Di-Me:* [49810-25-5].
$C_6H_{11}N_5$ M 153.186
Cryst. (C_6H_6). Mp 153-155°.

N^4,N^4-*Di-Me:* [24867-25-2].
$C_6H_{11}N_5$ M 153.186
Cryst. (EtOH). Mp 193-194.5°. pK_{a1} 7.21 (20°), pK_{a2} 0.68 (20°).

N^4,N^6-*Di-Me:*
$C_6H_{11}N_5$ M 153.186
Cryst. (as hydrochloride). Mp 326° (hydrochloride).

N^4,N^6-*Di-Et:*
$C_8H_{15}N_5$ M 181.240
Needles (C_6H_6). Mp 135.5-136°.

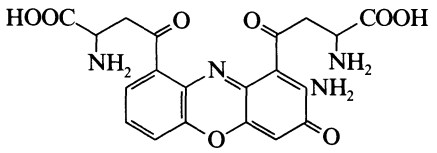
N^2,N^2,N^4,N^4-*Tetra-Me:* [3549-10-8].
$C_8H_{15}N_5$ M 181.240
Cryst. (C_6H_6). Mp 116-117°. pK_{a1} 7.18 (20°), pK_{a2} 0.81 (20°).

N^4,N^4,N^6,N^6-*Tetra-Me:* [24867-28-5].
$C_8H_{15}N_5$ M 181.240

Descr. by Roth *et al* but synth. apparently not publ.

Sadtler Standard Infrared Spectra, 22088 (*ir*)
Sadtler Standard NMR Spectra, 29686 (*pmr*)
Traube, W., *Chem. Ber.*, 1901, **34**, 3363 (*synth*)
Roth, B. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 1914 (N^4-Me, N^4,N^4-di-Me)
Forrest, H.S. *et al*, *J. Chem. Soc.*, 1951, **3** (N^4,N^6-di-Et)
Elion, G.B. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 4311 (N^4,N^6-di-Me)
Thompson, W.K., *J. Chem. Soc.*, 1962, 617 (N^2,N^2-di-Me, ir)
Roth, B. *et al*, *J. Org. Chem.*, 1970, **35**, 2696 (*derivs*, *props*, *uv*)
McCall, J.M. *et al*, *J. Org. Chem.*, 1975, **40**, 3304 (*oxides*)
Riand, J. *et al*, *Org. Magn. Reson.*, 1977, **9**, 572 (*cmr*, *pmr*)
Staedeli, W. *et al*, *Helv. Chim. Acta*, 1980, **63**, 504 (*N*-15 *nmr*)
Schwalbe, C.H. *et al*, *Acta Crystallogr.*, *Sect. B*, 1982, **38**, 1840 (*cryst struct*)
Wells, C.H.J., *Org. Magn. Reson.*, 1982, **20**, 274 (*pmr*, *derivs*)
Riand, J. *et al*, *J. Heterocycl. Chem.*, 1983, **20**, 1187 (*ms*)
Cowden, W.B., *Aust. J. Chem.*, 1984, **37**, 1195 (N^4-Et)
Narita, J. *et al*, *Chem. Pharm. Bull.*, 1985, **33**, 4928 (*use*)

α,α′,2-Triamino-γ,γ′,3-trioxo-3*H*-phenoxazine-1,9-dibutanoic acid, 9CI — T-80209

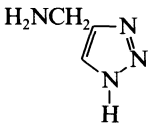


$C_{20}H_{18}N_4O_8$ M 442.384
Probable struct. Ommochrome pigment from the eyes and skin of cephalopods *Loligo vulgaris*, *Sepia officinalis* and *Octopus vulgaris*. Yellow. Insoluble. λ_{max} 420-440 nm. Readily cyclises to dihydroxanthommatin.

Bolognese, A. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1243 (*bibl*)

1*H*-1,2,3-Triazole-4-methanamine — T-80210

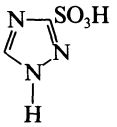
4(5)-Aminomethyl-1,2,3-triazole
[118724-05-3]



$C_3H_6N_4$ M 98.107
Cryst. (dioxan aq. or by subl.). Mp 206°.

Banert, K., *Chem. Ber.*, 1989, **122**, 911 (*synth*, *ir*, *pmr*, *cmr*)

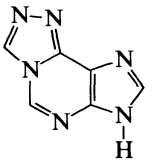
1,2,4-Triazole-3(5)-sulfonic acid — T-80211



$C_2H_3N_3O_3S$ M 149.130
Fluoride: [78201-15-7].
$C_2H_2FN_3O_2S$ M 151.121
Cryst. + $\frac{1}{2}$ H_2O (EtOH). Mp 68-70°.
Amide: [89517-96-4].
$C_2H_4N_4O_2S$ M 148.145
Mp 227-230°.

Hanna, N.B. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 1857.

1*H*-1,2,4-Triazolo[3,4-*i*]purine — T-80212

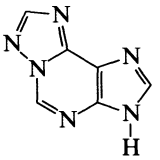


$C_6H_4N_6$ M 160.138
Cryst. (DMF). Mp >264°.

Temple, C. *et al*, *J. Org. Chem.*, 1965, **30**, 3601 (*synth*, *ir*, *uv*)

1*H*-1,2,4-Triazolo[5,1-*i*]purine, 9CI — T-80213

[4022-94-0]

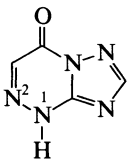


$C_6H_4N_6$ M 160.138
Cryst. (MeCN/MeOH aq.). Mp >250°.

Temple, C. *et al*, *J. Org. Chem.*, 1965, **30**, 3601 (*synth*, *ir*, *uv*)
Weimer, D.F. *et al*, *J. Org. Chem.*, 1974, **39**, 3438 (*synth*, *uv*, *ms*)
Hosmane, R.S. *et al*, *J. Org. Chem.*, 1988, **53**, 382 (*synth*, *pmr*)

[1,2,4]-Triazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one — T-80214

[57351-74-3]

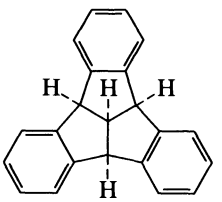


$C_4H_3N_5O$ M 137.101
Mp 236-238°.
1-Me: [59105-03-2].
$C_5H_5N_5O$ M 151.127
Mp 171-173°.
2-Me: [112298-55-2].
$C_5H_5N_5O$ M 151.127
Mp 211-214°. Zwitterionic.

Tennant, G. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1976, 421 (*synth*, *ir*, *pmr*, *uv*)
Farràs, J. *et al*, *J. Org. Chem.*, 1988, **53**, 887 (*synth*, *pmr*, *ir*, *cmr*)

Tribenzotriquinacene — T-80215

4b,8b,12b,12d-Tetrahydrodibenzo[2,3:4,5]pentaleno[1,6-ab]indene, 9CI
[120022-86-8]



$C_{22}H_{16}$ M 280.368
Long needles (xylene). Mp 390°. Forms a monoanion and a dianion.

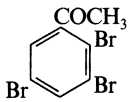
[120022-88-0, 120022-90-4]

Kuck, D. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 595 (*synth, pmr, uv*)

2′,3′,5′-Tribromoacetophenone T-80216

1-(2,3,5-Tribromophenyl)ethanone, 9CI

[116772-81-7]



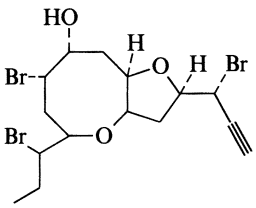
$C_8H_5Br_3O$ M 356.839

Pale reddish prisms (pet. ether). Mp 54-55°.

Tashiro, M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 179 (*synth, pmr, ms*)

3,6,13-Tribromo-4,10:9,12-diepoxy-14-pentadecyn-7-ol T-80217

Updated Entry replacing B-70195



$C_{15}H_{21}Br_3O_3$ M 489.041

Incorrect struct. originally assigned. Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ −8.2° (c, 0.09 in $CHCl_3$).

Ac: [94444-25-4]. *9-Acetoxy-3,10,13-tribromo-4,7:6,12-diepoxy-1-pentadecyne*

$C_{17}H_{23}Br_3O_4$ M 531.078

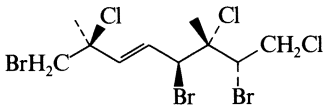
Metab. of red alga *L. obtusa*. Mobile oil. $[\alpha]_D$ −29.3° (c, 1.14 in $CHCl_3$).

Gonzalez, A.G. *et al*, *Tetrahedron*, 1984, **40**, 3443 (*isol*)

Norte, M. *et al*, *Tetrahedron*, 1989, **45**, 5987 (*struct*)

1,5,7-Tribromo-2,6,8-trichloro-2,6-dimethyl-3-octene T-80218

[119903-43-4]



$C_{10}H_{14}Br_3Cl_3$ M 480.291

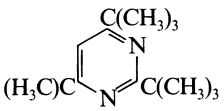
Constit. of *Plocamium hamatum*. Cryst. Mp 92.5-94°. $[\alpha]_D$ −118° (c, 0.017 in $CHCl_3$).

Coll, J.C. *et al*, *Aust. J. Chem.*, 1988, **41**, 1743 (*isol, cryst struct*)

2,4,6-Tri-*tert*-butylpyrimidine T-80219

2,4,6-Tris(1,1-dimethylethyl)pyrimidine, 9CI

[67490-21-5]



$C_{16}H_{28}N_2$ M 248.411

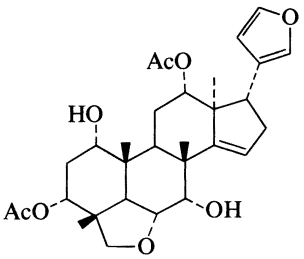
Cryst. (EtOH aq.). Mp 79-80°. pK_a 1.02 (H_2O, 25°).

B,HBF₄: Mp 200-201°.

van der Plas, H.C. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1978, **97**, 159.

Trichilinin T-80220

Updated Entry replacing T-60251



$C_{30}H_{40}O_8$ M 528.641

Constit. of *Trichilia roka*.

1-Ac:

$C_{32}H_{42}O_9$ M 570.678

Constit. of *Melia volkensii*. Cryst. (Me_2CO/hexane). Mp 114-116°.

1-O-Tigloyl:

$C_{35}H_{46}O_9$ M 610.743

Constit. of *M. volkensii*. Cryst. (Me_2CO/hexane). Mp 168-170°.

1-O-Cinnamoyl:

$C_{39}H_{46}O_9$ M 658.787

Constit. of *M. volkensii*. Cryst. (Me_2CO/hexane). Mp 134-136°.

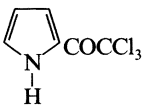
Nakatani, M. *et al*, *Heterocycles*, 1987, **26**, 43 (*isol, struct*)

Rajat, M.S. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 840 (*derivs*)

2-(Trichloroacetyl)pyrrole T-80221

2,2,2-Trichloro-1-(1H-pyrrol-2-yl)ethanone, 9CI. 2-Pyrrolyl trichloromethyl ketone

[35302-72-8]



$C_6H_4Cl_3NO$ M 212.462

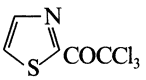
Tan solid (hexane). Mp 73-75°.

Org. Synth., 1971, **51**, 100 (*synth*)

2-(Trichloroacetyl)thiazole T-80222

2,2,2-Trichloro-1-(2-thiazolyl)ethanone, 9CI

[87636-20-2]



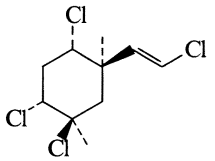
$C_5H_2Cl_3NOS$ M 230.501

Cryst. (Et_2O/hexane). Mp 62-64°.

Dondoni, A. *et al*, *J. Org. Chem.*, 1988, **53**, 1748 (*synth, ir, pmr, ms*)

1,2,4-Trichloro-5-(2-chloroethenyl)-1,5-dimethylcyclohexane T-80223

[119945-08-3]



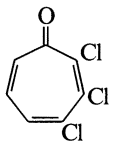
$C_{10}H_{14}Cl_4$ M 276.031
Constit. of *Plocamium hamatum*. Cryst. Mp 86-88°. $[\alpha]_D$ +9.4° (c, 0.01 in $CHCl_3$).

Coll, J.C. *et al*, *Aust. J. Chem.*, 1988, **41**, 1743 (*isol, cryst struct*)

2,3,4-Trichloro-2,4,6-cycloheptatrien-1-one, 9CI T-80224

2,3,4-Trichlorotropone

[114125-03-0]



$C_7H_3Cl_3O$ M 209.458
Pale yellow solid. Mp 88°. $Bp_{0.2}$ 120° (kugelrohr) .

Seitz, G. *et al*, *Synthesis*, 1987, 953 (*synth, ms, ir, uv, pmr, cmr*)

1,1,2-Trichloro-1,2-difluoroethane, 9CI T-80225

[354-15-4]

$Cl_2CFCHFCl$

$C_2HCl_3F_2$ M 169.385
Shows anaesthetic props. d_4^{20} 1.559. Bp 71-72.6°. n_D^{20} 1.3942 (1.3967).

Hauptschein, M. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3423 (*synth*)
Bindal, M.C. *et al*, *Azneim-Forsch*, 1980, **30**, 234 (*use, ir*)

1,2,2-Trichloro-1,1-difluoroethane, 9CI T-80226

[354-21-2]

$F_2CClCHCl_2$

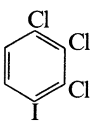
$C_2HCl_3F_2$ M 169.385
Shows anaesthetic props. Bp 71.9°.

[41834-16-6]

Heberling, J.W., *J. Org. Chem.*, 1958, **23**, 615 (*synth, ms*)
Fessenden, R.W. *et al*, *J. Chem. Phys.*, 1962, **37**, 1466 (*pmr, F-19 nmr*)
Hørnischer, R. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 81 (*raman*)
Chuvatken, N.N. *et al*, *Zh. Org. Khim.*, 1982, **18**, 946 (*synth*)

1,2,3-Trichloro-4-iodobenzene T-80227

[62720-28-9]



$C_6H_2Cl_3I$ M 307.344
Cryst. solid (pet. ether). Mp 66-66.5° (50-52°).

Bolton, R. *et al*, *J. Chem. Soc., Perkin Trans.* 2, 1977, 278 (*synth*)
Ghosh, T. *et al*, *J. Org. Chem.*, 1988, **53**, 3555 (*synth*)

1,1,1-Trichloro-2,2,3,3,3-pentafluoropropane, 9CI T-80228

Freon 215

[4259-43-2]

$F_3CCF_2CCl_3$

$C_3Cl_3F_5$ M 237.383
Solv. for disperse dyes, cleaning solv. Intermed. for fluorine-containing anaesthetics. d_4^{20} 1.637. Bp 70.5°, Bp ~72° . n_D^{20} 1.3527.

McBee, E.T. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 3149 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 1867 (*uv*)

1,1,3-Trichloro-1,2,2,3,3-pentafluoropropane, 9CI T-80229

[1652-81-9]

$FCl_2CF_2CClF_2$

$C_3Cl_3F_5$ M 237.383
Degreasing solvent. d_4^{25} 1.643. Mp −132.4°. Bp 72-73° (75°) . n_D^{25} 1.3578, n_D^{20} 1.3512.

Coffman, D.D. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 979 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
White, H.F., *Anal. Chem.*, 1966, **38**, 625 (*F nmr*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 1867 (*synth, ir, uv*)

1,2,2-Trichloro-1,1,3,3,3-pentafluoropropane, 9CI T-80230

[1599-41-3]

$F_3CCCl_2CClF_2$

$C_3Cl_3F_5$ M 237.383
d_4^{30} 1.644, d_4^{20} 1.668. Mp −4.5°. Bp 72°. n_D^{20} 1.3518.

Farah, B.S. *et al*, *J. Org. Chem.*, 1965, **30**, 1241 (*synth*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)

1,2,3-Trichloro-1,1,2,3,3-pentafluoropropane, 9CI T-80231

[76-17-5]

$F_2CClCClFCClF_2$

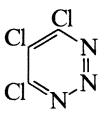
$C_3Cl_3F_5$ M 237.383
Liq. (glass at low temps.). d_4^{20} 1.663. Mp −141.3°, Mp −135.0° (dimorph.). Bp 72-73°. n_D^{20} 1.3512, n_D^{22} 1.350.

[28109-69-5]

Henne, A.H. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 130 (*synth*)
Miller, W.J. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 4164 (*synth, props*)
Fainberg, A.H. *et al*, *J. Org. Chem.*, 1965, **30**, 864 (*props*)
Paleta, O. *et al*, *Bull. Soc. Chim. Fr.*, 1986, 920 (*synth*)

Trichloro-1,2,3-triazine T-80232

[70674-51-0]

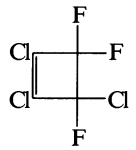


$C_3Cl_3N_3$ M 184.411
Mp 110-112°.

Gompper, R. *et al*, *Chem. Ber.*, 1979, **112**, 1529 (*synth*)

1,2,3-Trichloro-3,4,4-triflurorocyclobutene, 9CI **T-80233**

[3762-49-0]



$C_4Cl_3F_3$ M 211.397
d_4^{25} 1.59. Bp_{625} 95°. n_D^{25} 1.4153.

Park, J.D. *et al*, *J. Org. Chem.*, 1965, **30**, 400 (*synth, ir*)
Bauer, G. *et al*, *Z. Naturforsch., B*, 1979, **34**, 1249 (*synth*)

3-Tricosene, 9CI **T-80234**

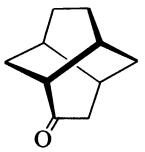
$H_3C(CH_2)_{18}CH{=}CHCH_2CH_3$

$C_{23}H_{46}$ M 322.616
Isol. from rose oil wax (*Rosa* sp.), prob. mostly as *Z*-form.

Wollrab, V. *et al*, *Collect. Czech. Chem. Commun.*, 1965, **30**, 1654 (*isol*)

Tricyclo[4.4.0.0^{3,8}]decan-4-one, 9CI **T-80235**

Updated Entry replacing T-20210
4-Twistanone
[13537-95-6]



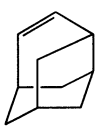
(+)-*form*

$C_{10}H_{14}O$ M 150.220
(+)-***form*** [25225-94-9]
$[\alpha]_D^{25}$ +295° (c, 0.518 in EtOH).
(−)-***form*** [74958-51-3]
Cryst. by subl. Mp 159-161°. $[\alpha]_D^{27}$ −270° (c, 0.97 in EtOH). Estimated optical purity 83%.
(±)-***form***
Mp 185-190°.
2,4-Dinitrophenylhydrazone: [13537-96-7].
Cryst. (H_2O). Mp 170-171°.

Gauthier, J. *et al*, *Can. J. Chem.*, 1967, **45**, 297 (*synth*)
Tichý, M., *Tetrahedron Lett.*, 1972, 2001 (*synth*)
Dodds, D.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 1080 (*synth*)
Nakazaki, M. *et al*, *J. Org. Chem.*, 1983, **48**, 2506 (*synth*)
Dodds, D.R. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 577 (*synth, ir, cmr*)

Tricyclo[4.3.1.0^{3,8}]dec-4-ene **T-80236**

*2,3,3a,4,5,7a-Hexahydro-2,5-methano-1*H*-indene, 9CI. Protoadamantene*
[29844-85-7]

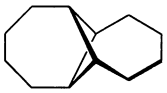


$C_{10}H_{14}$ M 134.221
Mp 183-185°.

Cupas, C.A. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 3237 (*synth*)
Black, R.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 972 (*synth, pmr*)
Cuddy, B.D. *et al*, *J. Chem. Soc. C*, 1971, 3173 (*synth*)
Boyd, J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1972, 2533 (*synth*)
Majerski, Z. *et al*, *Org. Mass Spectrom.*, 1977, **12**, 37 (*ms*)
Kropp, P.J. *et al*, *Tetrahedron Lett.*, 1978, 207.

Tricyclo[5.5.0.0^{2,8}]dodecane **T-80237**

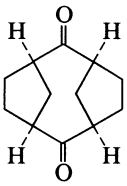
[61506-29-4]



$C_{12}H_{20}$ M 164.290
Solid. Mp <20°.

Gleiter, R. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5490 (*synth, ir, pmr, cmr*)

Tricyclo[6.2.1.1^{3,6}]dodecane-2,7-dione, 9CI **T-80238**

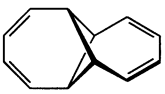


$C_{12}H_{16}O_2$ M 192.257
(***1α,3α,6α,8α***)-***form*** [113428-76-5]
Cryst. (EtOAc/hexane). Mp 192°.

Xu, C. *et al*, *Tetrahedron*, 1987, **43**, 2909 (*synth, cmr, cryst struct*)

Tricyclo[5.5.0.0^{2,8}]dodeca-3,5,9,11-tetraene **T-80239**

[61278-83-9]

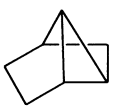


$C_{12}H_{12}$ M 156.227
Musty-smelling plates by subl. Mp 33.5-35.5°.

Dressel, J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5479 (*synth, ir, pmr, cmr, uv*)
Gleiter, R. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5490 (*pe, props*)

Tricyclo[3.2.0.0^{2,7}]heptane, 9CI **T-80240**

Tricyclo[4.1.0.0^{3,7}]heptane. Pseudonortricyclane
[279-18-5]



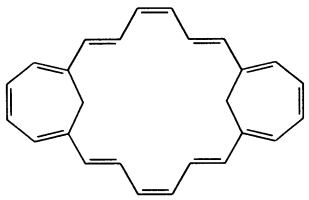
C_7H_{10} M 94.156

Moore, W.R. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2019 (*synth*)
Adam, W. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 6406 (*pmr, cmr, ir, ms*)

Tricyclo[18.4.1.1.^{8,13}]hexacosa-2,4,6,8,10,12,14,16,18,20,22,24-dodecaene, 9CI **T-80241**

1,6:13,18-Dimethano[24]annulene

[115351-49-0]



$C_{26}H_{24}$ M 336.476

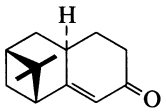
Black-brown needles (hexane/C_6H_6). Mp 200° dec. Paratropic.

Yamamoto, K. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 395 (*synth, uv, ir, pmr*)

Tricyclone **T-80242**

2,3,4,4a,5,6-Hexahydro-2,2-dimethyl-1,3-methanonaphthalen-7(1H)-one, 9CI. 10,10-Dimethyltricyclo[7.1.1.0^{2,7}]undec-2-en-4-one

[68433-81-8]



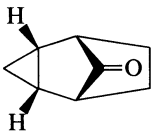
Absolute configuration

$C_{13}H_{18}O$ M 190.285

Perfumery chemical. d_4^{20} 1.015. $Bp_{0.01}$ 88-90°. $[\alpha]_D^{20}$ +40.4° (neat). Tricyclone is a proprietary name.

Bessière, Y. *et al*, *Nouv. J. Chim.*, 1978, **2**, 365 (*synth*)
Thomas, A.F. *et al*, *Helv. Chim. Acta*, 1981, **64**, 161 (*pmr, config*)

Tricyclo[3.2.1.0^{2,4}]octan-8-one **T-80243**



endo-form

$C_8H_{10}O$ M 122.166

endo-form [14224-86-3]

Solid by subl. Mp 71-72°.

exo-form [7076-83-7]

Bp_{17} 83-84°.

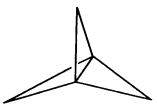
Tanida, H. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 1953 (*synth*)
Pincock, R.E. *et al*, *Tetrahedron Lett.*, 1967, 4759 (*uv, pmr*)
Haywood-Farmer, J.S. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 3020 (*synth, ir, pmr, ms*)
Kelly, D.P. *et al*, *J. Org. Chem.*, 1988, **53**, 2497 (*pmr, cmr*)

Tricyclo[1.1.1.0^{1,3}]pentane, 9CI **T-80244**

Updated Entry replacing T-50405

[1.1.1]Propellane

[35634-10-7]



C_5H_6 M 66.102

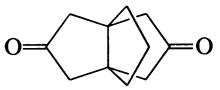
Remarkably stable, $t_{1/2}$ ~5 min. at 114°.

Wiberg, K.B. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 5239 (*synth, cmr, pmr, ms*)
Wiberg, K.B. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 7247 (*synth, struct*)
Hedberg, L. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 7257 (*struct*)
Belzner, J. *et al*, *Chem. Ber.*, 1989, **122**, 397.

Tricyclo[3.3.3.0^{1,5}]undecane-3,7-dione **T-80245**

1H,4H-3a,6a-Propanopentalene-2,5(3H,6H)-dione, 9CI. [3.3.3]Propellane-3,7-dione

[21170-73-0]



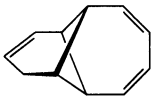
$C_{11}H_{14}O_2$ M 178.230

Cryst. (MeOH). Mp 224° (185-187°).

Weiss, U. *et al*, *Tetrahedron Lett.*, 1968, 4885 (*synth*)
Weber, R.W. *et al*, *Can. J. Chem.*, 1978, **56**, 189 (*synth*)
Mitschka, R. *et al*, *Tetrahedron*, 1981, **37**, 4521 (*synth*)
Quast, H. *et al*, *Chem. Ber.*, 1989, **122**, 523 (*synth, pmr*)

Tricyclo[5.4.0.0^{2,8}]undeca-3,5,9-triene, 9CI **T-80246**

[115462-81-2]



$C_{11}H_{12}$ M 144.216

Volatile liq.

Gleiter, R. *et al*, *J. Org. Chem.*, 1988, **53**, 3912 (*synth, pmr, cmr, ir, uv*)

3,5,11-Tridecadiene-7,9-diyne-1,2-diol **T-80247**

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH(OH)CH_2OH$

$C_{13}H_{14}O_2$ M 202.252

(E,E,E)-form

From *Centaurea ruthenica* and *Serratula wolfii*. Cryst. ($CHCl_3$). Mp 117°. $[\alpha]_D^{24}$ −1.7° (MeOH).

Di-Ac: [60032-82-8].

Cryst. (Et_2O/cyclohexane). Mp 57°. $[\alpha]_D^{24}$ +94.5° (Me_2CO).

Bohlmann, F. *et al*, *Chem. Ber.*, 1961, **94**, 3179; 1962, **95**, 2939; 1976, **109**, 2291 (*isol, synth, uv, ir*)

5,10,12-Tridecadiene-2,8-diyne-4,7-thione **T-80248**

7,10-Dithioxo-1,3,8-tridecatriene-5,11-diyne

$H_3CC{\equiv}CC(S)CH{=}CHC(S)C{\equiv}CCH{=}CHCH{=}CH_2$

$C_{13}H_{10}S_2$ M 230.354

(3E,8Z)-form

Isol. from roots of *Rudbeckia bicolor* and *Melampodium* spp. Red oil. λ_{max} 263 infl. (ϵ 14050), 351 (14300), 488 nm (2930) (pet. ether).

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 3081 (*isol, uv, ir, pmr, ms*)

8,10-Tridecadiene-4,6-diyn-1-ol, 9CI **T-80249**

$H_3CCH_2CH{=}CHCH{=}CHC{\equiv}CC{\equiv}CCH_2CH_2CH_2OH$

$C_{13}H_{16}O$ M 188.269

(E,E)-form

Dihydroaethusanol B

Isol. from above-ground parts of *Aethusa cynapium*.
p-*Phenylazobenzoyl:* Mp 99°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 2598.

1,11-Tridecadiene-3,5,7,9-tetrayne, 9CI T-80250

[2345-16-6]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CH_2$

$C_{13}H_8$ M 164.206

(E)-form [26130-86-9]

Trace constituent of roots of *Zoegea baldschuanica* and *Triticum aestivum*. Isol.from roots of *Dahlia* sp., from roots of *Bidens graveolens* and other *B*.spp., from seedlings of *Carthamus tinctorius* and from *Coreopsis* sp. Widespread minor constit. of the Compositae. Pale yellow needles (pentane). Dec. without melting >40°. Rapidly becomes brown in diffused daylight even at −5°.

(Z)-form [59950-58-2]

Isol. from roots of *D.* sp., from *Coreopsis* sp. and *Carthamus tinctorius*. Liq.

Sorensen, J.S. *et al*, *Acta Chem. Scand.*, 1954, **8**, 1741 (*isol, ir*)
Jones, E.R.H. *et al*, *J. Chem. Soc.*, 1958, 1054 (*synth, uv, ir, glc*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 1315; 1964, **97**, 1193, 2583; 1965, **98**, 872, 1228; 1966, **99**, 3201, 3433, 3544; 1971, **104**, 961 (*isol, struct, occur*)
Schulte, K.E. *et al*, *Phytochemistry*, 1965, **4**, 481 (*isol*)
Chin, C. *et al*, *J. Chem. Soc. C*, 1970, 314 (*isol*)
Bedford, C.T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 735 (*isol*)
Binder, R.G. *et al*, *Phytochemistry*, 1978, **17**, 315 (*isol, ms, uv, pmr*)
Bohlmann, F. *et al*, *Phytochemistry*, 1983, **22**, 1281 (*isol*)

1,12-Tridecadiene-3,5,7,9-tetrayne, 9CI T-80251

[80453-50-5]

$H_2C{=}CHCH_2C{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CH_2$

$C_{13}H_8$ M 164.206
Isol. from *Calea* sp.

Bohlmann, F. *et al*, *Phytochemistry*, 1981, **20**, 1643 (*isol, struct*)

1,3-Tridecadiene-5,7,9,11-tetrayne, 9CI T-80252

[18668-88-7]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH{=}CH_2$

$C_{13}H_8$ M 164.206

(E)-form [3760-28-9]

Trace constituent of roots of *Rudbeckia amplexicaulis*, *R. bicolor*, *Fluorensia heterolepsis*,*Scaevola lobelia*, *Helichrysum vestitum* and *Arnica chamissonis*. Unstable cryst. (pet. ether). λ_{max} 273, 289.5, 311, 331, 355.5, 382 nm (Et_2O).

1,2-Epoxide: ***2-(1-Undecen-3,5,7,9-tetraynyl)oxirane.*** *1,2-Epoxy-3-tridecene-5,7,9,11-tetrayne*
$C_{13}H_8O$ M 180.206
Isol. from *Carthamus*, *Centaurea* and *Silybium* spp. Cryst. Mp 95.5-97°. $[\alpha]_D$ +75.1° ($CHCl_3$).

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 809, 2125; 1965, **98**, 3081; 1966, **99**, 3201, 3433, 3544; 1975, **108**, 433 (*isol, uv, ir, synth*)
Schulte, K.E. *et al*, *J. Nat. Prod.* (*Lloydia*), 1969, **32**, 360 (*isol, struct*)
Bohlmann, F. *et al*, *Phytochemistry*, 1979, **18**, 1189; 1980, **19**, 331 (*isol*)

2,12-Tridecadiene-4,6,8,10-tetrayn-1-ol, 9CI T-80253

[20252-36-2]

$H_2C{=}CH^{11}C{\equiv}^{10}CC{\equiv}CC{\equiv}CCH{=}CHCH_2OH$

$C_{13}H_8O$ M 180.206
Isol. from *Bidens* spp., *Cosmos diversifolius* and *Coreopsis tinctoria*. Cryst. (pet. ether). Mp 41-42°.

Ac: [20252-35-1]. *1-Acetoxy-2,12-tridecadiene-4,6,8,10-tetrayne*
$C_{15}H_{10}O_2$ M 222.243
Isol. from *Coreopsis* sp., *B.* sp., *Cosmos* sp. and *Leptosyne calliopsidea*. Amorph. λ_{max} 270, 287, 314, 336, 361, 391 nm.

10,11-Dihydro(E-)*: 2,10,12-Tridecatriene-4,6,8-triyn-1-ol, 9CI*
$C_{13}H_{10}O$ M 182.221
Isol. from *Cosmos sulphureus*, *C. hybridus* and *Coreopsis tinctoria*. Cryst. (Et_2O/pet. ether). Mp 100° dec.

[26130-87-0, 26130-89-2]

Bohlmann, F. *et al*, *Chem. Ber.*, 1962, **95**, 1315; 1964, **97**, 1193, 2135, 2583; 1965, **98**, 1228; 1966, **99**, 1223.

3,11-Tridecadiene-5,7,9-triyne-1,2-diol, 9CI T-80254

Safynol

[65398-35-8]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH(OH)CH_2OH$

$C_{13}H_{12}O_2$ M 200.237

(2R,3E,11E)-form [27978-14-9]

Isol. from *Centaurea* spp., *Bidens* spp. and fungus-infected safflower (*Carthamus tinctorius*). Antifungal, antibiotic phytoalexin. Cryst. ($CHCl_3$/hexane). Mp 122.5-123.5° (112°). $[\alpha]_D^{20}$ −17°. Stable in dark at −18°, resinifies in air.

2-Ac: Cryst. (pet. ether/Et_2O). Mp 86°. $[\alpha]_D^{21}$ +39° ($CHCl_3$).

Di-Ac:
$C_{17}H_{16}O_4$ M 284.311
Occurs naturally. Cryst. (Et_2O or pet. ether/Et_2O). Mp 64° (80°). $[\alpha]_D^{20}$ +102.2° ($CHCl_3$).

(2S,3E,11E)-form [65207-93-4]
$[\alpha]_D^{22.5}$ +18.4°, $[\alpha]_D^{23}$ +30.8° (MeOH).

Bohlmann, F. *et al*, *Chem. Ber.*, 1958, **91**, 1642, 3179 (*isol, ir, synth, uv*)
Allen, E.H. *et al*, *Phytochemistry*, 1971, **10**, 1579 (*isol, ir, ms, uv*)
Nakada, H. *et al*, *Agric. Biol. Chem.*, 1977, **41**, 1761 (*isol, synth, ir, ord, pmr, uv*)
Jente, R. *et al*, *Phytochemistry*, 1979, **18**, 829 (*pmr*)
MacRae, W.D. *et al*, *Experientia*, 1980, **36**, 1096 (*pharmacol*)

1,6-Tridecadiene-3,9,11-triyne-5,8-dithione T-80255

5,8-Dithioxo-1,6-tridecadiene-3,9,11-triyne

$H_3CC{\equiv}CC{\equiv}CC(S)CH{=}CHC(S)C{\equiv}CCH{=}CH_2$

$C_{13}H_8S_2$ M 228.338

(Z)-form

Isol. from *Eriophyllum caespitosum*. Red oil. λ_{max} 230 (ϵ 23200), 353 (12,500), 499 nm (3070) (pet. ether).

Mortensen, J.T. *et al*, *Acta Chem. Scand.*, 1964, **18**, 2392 (*isol, uv, ir, pmr*)
Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 3081.

5,12-Tridecadiene-2,8,10-triyne-4,7-dithione T-80256

7,10-Dithioxo-1,8-tridecadiene-3,5,11-triyne

$H_3CC{\equiv}CC(S)CH{=}CHC(S)C{\equiv}CC{\equiv}CCH{=}CH_2$

$C_{13}H_8S_2$ M 228.338

(Z)-form

Isol. from roots of *Ambrosia elatior*, also in other *A.* spp., *Schkuhria* spp. and *Iva xanthiifolia*. Red oil. λ_{max} 231 (ϵ 24100), 340 (12700), 496 nm (3000) (hexane).

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 3081 (*isol, uv, ir, pmr, ms, struct*)

3,11-Tridecadiene-5,7,9-triyne-1,2,13-triol T-80257

$HOCH_2CH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH(OH)CH_2OH$

$C_{13}H_{12}O_3$ M 216.236

(E,E)-form

Isol. from above ground parts of *Bidens bipinnata*. Cryst. (Et_2O/pet. ether). Polymerises above 100°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1228 (*isol, uv, ir, struct*)

3,5-Tridecadiene-7,9,11-triyn-1-ol, 9CI T-80258

[56319-28-9]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH_2CH_2OH$

$C_{13}H_{12}O$ M 184.237

(E,E)-form [3513-72-2]

Isol. from above ground parts of *Chrysanthemum ircutianum*. Cryst. (pet. ether/Et_2O). Mp 102° (95-97°).

Ac:

$C_{15}H_{14}O_2$ M 226.274

Isol. from above ground parts of *C. ircutianum*.

3-Methylbutanoyl:

$C_{18}H_{20}O_2$ M 268.355

Isol. from roots of *C. leucanthemum*.

(3E,5Z)-form [75911-03-4]

Isol. from *Leucanthemum* sp.

Bohlmann, F. *et al*, *Chem. Ber.*, 1961, **94**, 3193; 1965, **98**, 2596 (*isol, uv, synth, deriv*)
Wrang, P.A. *et al*, *Phytochemistry*, 1975, **14**, 1027 (*isol*)
Bohlmann, F. *et al*, *Phytochemistry*, 1980, **19**, 841 (*isol*)

3,5,7,9,11-Tridecapentayne-1,2-diol T-80259

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH(OH)CH_2OH$

$C_{13}H_8O_2$ M 196.205

Isol. from above-ground parts of *Bidens leucantha*. Unstable light-yellow cryst. (Et_2O/pet. ether).

Di-Ac: [3420-89-1].

Yellowish cryst. (pet. ether). Mp 90° dec. $[\alpha]_D^{25}$ +52.5° (c, 0.19 in Et_2O).

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1228 (*isol, uv, ir, ord, struct*)

2,8,10,12-Tridecatetraene-4,6-diyn-1-ol, 9CI T-80260

$H_2C{=}CHCH{=}CHCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH_2OH$

$C_{13}H_{12}O$ M 184.237

(all-E)-form [15427-16-4]

Isol. from roots of *Carlina vulgaris*. Leaflets (Et_2O/pet. ether). Mp 86°.

Ac: 1-Acetoxy-2,8,10,12-tridecatetraene-4,6-diyne

$C_{15}H_{14}O_2$ M 226.274

Isol. from *Bidens ferulaefolia*, *Coreopsis tinctoria* and roots of *Carlina vulgaris*. Cryst. (pet. ether). Mp 31°.

(2Z,8E,10E)-form [75627-99-5]

Isol. from *Tetragonotheca helianthoides*.

Bohlmann, F. *et al*, *Chem. Ber.*, 1964, **97**, 1193; 1966, **99**, 1223; 1967, **100**, 1507 (*isol, uv, ir, pmr, deriv*)
Bedford, C.T. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 735 (*isol*)
Seaman, F.C. *et al*, *Phytochemistry*, 1980, **19**, 583 (*isol*)

11-Tridecene-3,5,7,9-tetrayne-1,2-diol, 9CI T-80261

Dehydrosafynol

[1540-85-8]

$H_3CCH{=}CH(C{\equiv}C)_4CH(OH)CH_2OH$

$C_{13}H_{10}O_2$ M 198.221

(E)-form

Isol. from above-ground parts of *Bidens bipinnata*. Highly antifungal. No opt. rotn. reported.

Di-Ac: [1593-79-9].

Light-yellow cryst. (pet. ether). Mp 61°, Mp 88°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1228; 1967, **100**, 1209 (*isol, uv, ir, pmr, struct, synth*)

11-Tridecene-3,5,7,9-tetrayne-1,2,13-triol T-80262

$HOCH_2CH{=}CH(C{\equiv}C)_4CH(OH)CH_2OH$

$C_{13}H_{10}O_3$ M 214.220

(E)-form

Isol. from above ground parts of *Bidens bipinnata*. Unstable cryst. (Et_2O/pet. ether). Polymerises above 100°.

Tri-Ac: Yellowish oil.

Bohlmann, F. *et al*, *Chem. Ber.*, 1965, **98**, 1228 (*isol, uv, ir, pmr, struct*)

6-Tridecen-1-ol T-80263

$H_3C(CH_2)_5CH{=}CH(CH_2)_4CH_2OH$

$C_{13}H_{26}O$ M 198.348

(E)-form [37011-92-0]

Liq. $Bp_{0.3}$ 96-97°.

Voaden, D.J. *et al*, *J. Med. Chem.*, 1972, **15**, 619 (*synth*)
Svirskaya, P.I. *et al*, *J. Chem. Eng. Data*, 1979, **24**, 152.
Brown, H.C. *et al*, *J. Org. Chem.*, 1988, **53**, 246 (*synth, ir, pmr, cmr*)

3-Tridecyn-1-ol, 9CI T-80264

[54373-82-9]

$H_3C(CH_2)_8C{\equiv}CCH_2CH_2OH$

$C_{13}H_{24}O$ M 196.332

Oil. Mp 21.5-22°. $Bp_{0.6}$ 119-121°. n_D^{23} 1.4579.

Gilman, N.N. *et al*, *Chem. Phys. Lipids*, 1974, **13**, 239 (*synth*)
Bestmann, H.G. *et al*, *Justus Liebigs Ann. Chem.*, 1987, 417 (*synth, pmr, ir, ms*)
Mori, K. *et al*, *Justus Liebigs Ann. Chem.*, 1988, **8**, 807 (*synth, ir, pmr*)

6-Tridecyn-1-ol, 9CI T-80265

[37011-88-4]

$H_3C(CH_2)_3C{\equiv}C(CH_2)_4CH_2OH$

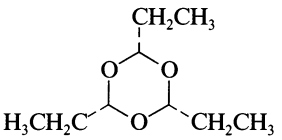
$C_{13}H_{24}O$ M 196.332

Oil. $Bp_{0.1}$ 104-105° (107-109°) . n_D^{25} 1.4608.

Voaden, D.J. *et al*, *J. Med. Chem.*, 1972, **15**, 619 (*synth*)
Svirskaya, P.A. *et al*, *J. Chem. Eng. Data*, 1979, **24**, 152 (*synth*)
Brown, H.C. *et al*, *J. Org. Chem.*, 1986, **57**, 4518 (*synth*)

2,4,6-Triethyl-1,3,5-trioxane, 9CI T-80266

Propionaldehyde trimer. Parapropionaldehyde. Parapropanal
[2396-42-1]



$C_9H_{18}O_3$ M 174.239
Normally consists exclusively of the 2α,4α,6α-form. Synthetic onion aroma. Colourless or yellowish oil. Spar. sol. H_2O, sol. EtOH, Et_2O. Fp −20°. Bp_{773} 172-173°, Bp_{10} 57-57.5° (60.5-61°) . n_D^{21} 1.4188. Reverts to monomer on treatment with dilute acid.

[1499-04-3]

Meier, R. *et al*, *Chem. Ber.*, 1957, **90**, 2344 (*synth*)
Blanc, P.-Y. *et al*, *Helv. Chim. Acta*, 1964, **47**, 567 (*synth, props, uv*)
Jungnickel, J.L. *et al*, *J. Mol. Spectrosc.*, 1965, **16**, 135 (*pmr, config*)
Ward, W.R. *et al*, *Spectrochim. Acta*, 1965, **2**, 1311 (*ir, raman*)
Seebald, H.J. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1973, **306**, 393 (*synth, ir, glc*)
Krasnov, V.L. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1983, **53**, 2135 (*synth, nmr*)
Abdelhader, M. *et al*, *Macromolecules*, 1987, **20**, 949 (*synth, pmr*)

Trifluoroacetic acid, 9CI, 8CI T-80267

Updated Entry replacing T-20220
Trifluoroethanoic acid
[76-05-1]

CF_3COOH

$C_2HF_3O_2$ M 114.024
Strong acid used in synthesis. Misc. H_2O. Fp −15.3°. Bp 70.5-72°. pK_a 0.23 (25°, H_2O).

▷ Mod. toxic, causes severe burns. AJ9625000.

Me ester: [431-47-0].
$C_3H_3F_3O_2$ M 128.051
Trifluoroacetylating agent for NH_2 groups. Liq. Bp 43-44°.

Et ester: [383-63-1].
$C_4H_5F_3O_2$ M 142.077
Liq. Bp 60-62°.

tert-*Butyl ester:* [400-52-2].
$C_6H_9F_3O_2$ M 170.131
Bp 83°.

Ph ester: [500-73-2]. *Phenyl trifluoroacetate*
$C_8H_5F_3O_2$ M 190.121
Reagent used to prepare *N*-trifluoroacetyl derivs. of amino acids etc. Bp 148-149°.

Amide: [354-38-1]. *Trifluoroacetamide*
$C_2H_2F_3NO$ M 113.039
Cryst. ($CHCl_3$). Mp 73.5-74.5°.

Anhydride: [407-25-0].
$C_4F_6O_3$ M 210.033
Trifluoroacetylating agent with several other synthetic uses. Bp 39.5°.

▷ Mod. toxic, causes severe burns. Reacts explosively with DMSO. AJ9800000.

Gilman, H. *et al*, *J. Am. Chem. Soc.*, 1943, **65**, 1458 (*amide, Et ester*)
Allen, D.R., *J. Org. Chem.*, 1961, **26**, 923 (*synth, props*)
U.S. Pat., 3 162 633, (1965); *CA*, **62**, 7780 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 850; 1975, **5**, 57; 1979, **7**, 246, 389; 1980, **8**, 503.
Berney, C.V., *J. Am. Chem. Soc.*, 1973, **95**, 708 (*spectra*)
Effenberger, F. *et al*, *Chem. Ber.*, 1980, **113**, 2100 (*tert*-Butyl ester)
Roberts, D.D. *et al*, *J. Org. Chem.*, 1988, **53**, 2573 (*amide*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 225, 396.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 1055.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 520.

1,1,2-Trifluoro-1,3-butadiene, 9CI T-80268

[565-65-1]

$F_2C{=}CFCH{=}CH_2$

$C_4H_3F_3$ M 108.063
Reagent for synth. of functionalised monofluoroalkene systems. Forms polymers with many substances. Volatile liq. or gas. Bp_{585} 0.5°.

Park, J.D. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 59 (*synth*)
Matsuo, N. *et al*, *J. Org. Chem.*, 1988, **53**, 2304 (*synth, pmr, F nmr, use*)

Trifluorobutanedioic acid, 9CI T-80269

Trifluorosuccinic acid, 8CI
[664-66-4]

$HOOCCF_2CHFCOOH$

$C_4H_3F_3O_4$ M 172.060

(±)-***form***
Cryst. Mp 111-112°.

*Anhydride: 3,3,4-Trifluoro-dihydro-2,5(2*H*,5*H*)-furandione*
$C_4HF_3O_3$ M 154.045
Bp 122-124°.

Diamide:
$C_4H_5F_3N_2O_2$ M 170.091
Cryst. (H_2O). Mp 195-197°.

Raasch, M.S. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 2678 (*synth*)

4,4,4-Trifluorobutanoic acid T-80270

[406-93-9]

$F_3CCH_2CH_2COOH$

$C_4H_5F_3O_2$ M 142.077
Mp 33.2°. Bp_{18} 78.0°, Bp 166.6°.

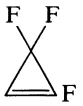
Chloride:
$C_4H_4ClF_3O$ M 160.523
Bp_{745} 103°.

Amide:
$C_4H_6F_3NO$ M 141.093
Cryst. Mp 136.4°.

McBee, E.T. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 2910 (*synth*)
Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 2323; 1955, **77**, 1901 (*derivs, props*)

1,3,3-Trifluorocyclopropene, 9CI T-80271

[35305-22-7]



C_3HF_3 M 94.036
Bp 6°.

Craig, N.C. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 180; 1975, **31**, 1463 (*synth, ir, ms, raman*)
Craig, N.C. *et al*, *J. Phys. Chem.*, 1985, **89**, 100.

1,1,1-Trifluoro-3,3-dimethyl-2-butanone T-80272

tert-*Butyl trifluoromethyl ketone*

$F_3CCOC(CH_3)_3$

$C_6H_9F_3O$ M 154.132
Liq. Bp 69-70°.

Dishart, K.T. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 2268 (*synth*)
Sykes, A. *et al*, *J. Chem. Soc.*, 1956, 835 (*synth*)
Feigl, D.M. *et al*, *J. Org. Chem.*, 1968, **33**, 4242 (*synth*)
Roberts, D.D. *et al*, *J. Org. Chem.*, 1988, **53**, 2573 (*synth*)

1,1,1-Trifluoroethane T-80273

Methylfluoroform

[420-46-2]

F_3CCH_3

$C_2H_3F_3$ M 84.041
Anaesthetic. d_4^{50} 1.176. Mp −111.3°. −47° to −46° .

▷ Flammable.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 889 (*synth*)
McBee, E.T. *et al*, *Ind. Eng. Chem.*, 1947, **39**, 409 (*props, synth*)
Whalley, W.B., *J. Soc. Chem. Ind., London*, 1947, **66**, 427 (*synth*)
Thompson, H.W. *et al*, *J. Chem. Soc.*, 1948, 1428 (*ir*)
Mohler, F.L. *et al*, *J. Chem. Phys.*, 1954, **22**, 394 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd *Ed.*, 1978-1984, *Wiley, NY*, 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 857; **11**, 65.
Buerger, H. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 7 (*ir, raman, pmr*)
Eujen, R. *et al*, *J. Fluorine Chem.*, 1983, **22**, 263 (*F*-19 *nmr*)

Trifluoroethene, 9CI T-80274

Trifluoroethylene

[359-11-5]

$F_2C{=}CHF$

C_2HF_3 M 82.025
Monomer for plastics. Gas. −61° to −60°, Bp_{628} −56° .

▷ Flammable.

Crosse, A.V. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 2289 (*synth*)
Craig, N.C. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 3047 (*synth*)
Tikhomirov, M.V. *et al*, *Zh. Fiz. Khim.*, 1967, **41**, 1065 (*ms*)
Hudlicky, M., *Chemistry of Organic Fluorine Compounds*, Wiley, London, 2nd ed., 1976, 603.
Galabov, B. *et al*, *J. Chem. Phys.*, 1979, **71**, 4716 (*ir*)
Bien, G. *et al*, *Chem. Phys.*, 1981, **60**, 61 (*pe, uv*)
Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co Ltd, Japan,, 1988, 090, 091 (*F-nmr, pmr*)

(Trifluoroethenyl)benzene, 9CI T-80275

α,β,β-Trifluorostyrene. (Trifluorovinyl)benzene. Trifluorophenylethylene

[447-14-3]

$PhCF{=}CF_2$

$C_8H_5F_3$ M 158.123
Forms polymers with many materials. Liq. Bp_{44} 59°.

Dixon, S., *J. Org. Chem.*, 1956, **21**, 400 (*synth*)
Heinze, P.L. *et al*, *J. Org. Chem.*, 1988, **53**, 2714 (*synth, ir, ms, pmr, cmr, F*-19 *nmr*)

1,1,1-Trifluoro-2-iodoethane, 8CI T-80276

2,2,2-Trifluoroethyl iodide

[353-83-3]

F_3CCH_2I

$C_2H_2F_3I$ M 209.938
Shows anaesthetic props. d_4^{25} 2.142. Bp 54-55°. n_D^{25} 1.3980.

[93347-76-3]

Haszeldine, R.N., *J. Chem. Soc.*, 1953, 2622 (*uv*)
Hauptschein, M. *et al*, *J. Org. Chem.*, 1958, **23**, 322 (*synth, ir*)
Chambers, R.D. *et al*, *J. Chem. Soc.*, 1961, 3779 (*synth*)
Harnish, D.F. *et al*, *Appl. Spectrosc.*, 1970, **24**, 28 (*ir*)
Boschi, R.A. *et al*, *Mol. Phys.*, 1972, **24**, 735 (*uv*)
Lopata, A.D. *et al*, *J. Raman Spectrosc.*, 1977, **6**, 61 (*raman*)

1,1,1-Trifluoro-2-methoxyethane, 9CI T-80277

Methyl 2,2,2-trifluoroethyl ether, 8CI

[460-43-5]

F_3CCH_2OMe

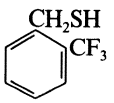
$C_3H_5F_3O$ M 114.067
Shows weak anaesthetic props. d_4^3 1.166. Bp_{746} 31.2°, Bp 31-32°. n_D^3 1.2942.

Robbins, B.H., *J. Pharmacol.*, 1946, **86**, 197 (*pharmacol*)
Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 4378 (*synth*)
Li, Y.S. *et al*, *J. Phys. Chem.*, 1987, **91**, 1334 (*ir, raman*)
Loehr, D.T. *et al*, *J. Fluorine Chem.*, 1988, **39**, 288.

2-(Trifluoromethyl)benzenemethanethiol, 9CI T-80278

(α,α,α-Trifluoro-o-tolyl)methanethiol, 8CI. o-(Trifluoromethyl)-α-toluenethiol. 2-(Trifluoromethyl)benzylmercaptan. 1-(Mercaptomethyl)-2-(trifluoromethyl)benzene

[26039-98-5]



$C_8H_7F_3S$ M 192.204
d_4^{25} 1.30. Bp_{13} 75°.

Belinskaya, R.V. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1970, **6**, 141 (*synth*)

3-(Trifluoromethyl)benzenemethanethiol, 9CI T-80279

(α,α,α-Trifluoro-m-tolyl)methanethiol, 8CI. 3-(Trifluoromethyl)benzylmercaptan. m-(Trifluoromethyl)-α-toluenethiol. 1-(Mercaptomethyl)-3-(trifluoromethyl)benzene

[25697-55-6]

$C_8H_7F_3S$ M 192.204
Liq. Bp_8 69-70°, $Bp_{2.1-2.2}$ 55°.

Paquette, L.A. *et al*, *J. Org. Chem.*, 1968, **33**, 1080 (*synth*)
Lombardino, J.G. *et al*, *J. Med. Chem.*, 1970, **13**, 206 (*synth*)

4-(Trifluoromethyl)benzenemethanethiol, 9CI **T-80280**

(α,α,α-*Trifluoro*-p-*tolyl*)*methanethiol, 8CI. 4-(Trifluoromethyl)benzyl mercaptan.* p-(*Trifluoromethyl*)-α-*toluenethiol. 1-(Mercaptomethyl)-4-(trifluoromethyl)benzene*

[108499-24-7]

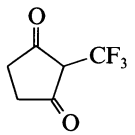
$C_8H_7F_3S$ M 192.204

Oil.

Buchwald, S.L. *et al, J. Am. Chem. Soc.*, 1988, **110**, 3171 (*synth, pmr, cmr, ir*)

2-Trifluoromethyl-1,3-cyclopentanedione, 9CI **T-80281**

[89049-67-2]



$C_6H_5F_3O_2$ M 166.099

Intermed. for steroid synth. Mp ~150° dec.

Blazejewski, J.C. *et al, Synthesis*, 1985, 1120 (*synth, ir, pmr, cmr, F-19 nmr*)

Blazejewski, J.C. *et al, J. Chem. Soc., Perkin Trans.* 1, 1986, 337.

3,3,3-Trifluoropropanal, 9CI **T-80282**

3,3,3-Trifluoropropionaldehyde

[460-40-2]

F_3CCH_2CHO

$C_3H_3F_3O$ M 112.051

Liq. d_4^{20} 1.37. Bp_{745} 56.0-56.5°.

2,4-Dinitrophenylhydrazone: Cryst. (EtOH aq.). Mp 150.2-150.8°.

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1950, **72**, 3370 (*synth*)

3,3,3-Trifluoro-1-propanamine, 9CI **T-80283**

3-Amino-1,1,1-trifluoropropane

[460-39-9]

$F_3CCH_2CH_2NH_2$

$C_3H_6F_3N$ M 113.082

Liq. d_4^{30} 1.16. Bp_{744} 67.8°.

B,HCl: Mp 222-225°.

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1955, **77**, 1901 (*synth*)

Hoffman, R.V. *et al, J. Am. Chem. Soc.*, 1988, **110**, 4019 (*synth*)

3,3,3-Trifluoropropanoic acid **T-80284**

β,β,β-Trifluoropropionic acid

[2516-99-6]

F_3CCH_2COOH

$C_3H_3F_3O_2$ M 128.051

Mp 9.7°. Bp_{746} 144.8°.

NH_4 salt: Bp_{21} 136° subl.

Aniline salt: Cryst. (EtOH). Mp 116°.

S-*Benzylthiouronium salt:* Cryst. (EtOH). Mp 176°.

Me ester: [18830-44-9].

$C_4H_5F_3O_2$ M 142.077

Bp 95-96°.

Et ester: [352-23-8].

$C_5H_7F_3O_2$ M 156.104

Bp 97-98°, Bp_{12} 50°.

Chloride:

$C_3H_2ClF_3O$ M 146.496

Bp_{745} 70.3°.

Amide:

$C_3H_4F_3NO$ M 127.066

Solid. Mp 108.8°. Bp_{12} 130° subl. . Deliquescent.

Anilide:

$C_9H_8F_3NO$ M 203.163

Cryst. (EtOH). Mp 118°.

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1951, **73**, 2323 (*props*)

Brown, F. *et al, J. Chem. Soc.*, 1953, 2087 (*synth, derivs*)

Kocharyan, S.T. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1967, 1847 (*esters, ir, pmr*)

2,4,6-Trihydroxybenzophenone, 8CI **T-80285**

Updated Entry replacing T-30274

(*2,4,6-Trihydroxyphenyl*)*phenylmethanone, 9CI. Phlorbenzophenone*

[3555-86-0]

$C_{13}H_{10}O_4$ M 230.220

Yellow cryst. + $1H_2O$ (H_2O). Mp 165°.

2-Me ether: [81525-12-4]. *2,4-Dihydroxy-6-methoxybenzophenone. Isocotoin*

$C_{14}H_{12}O_4$ M 244.246

Yellow needles. Mp 162°.

4-Me ether: [479-21-0]. *2,6-Dihydroxy-4-methoxybenzophenone.* ***Cotoin***

$C_{14}H_{12}O_4$ M 244.246

Occurs in Coto rind (*Nectandra coto*). Also from wood of *Aniba duckei*. Yellowish cryst. (H_2O). Mp 130-131°. Reduces Fehling's soln. and $NH_3.AgNO_3$ slowly in the cold.

▷ DJ1050000.

2,4-Di-Me ether: [34425-64-4]. *2-Hydroxy-4,6-dimethoxybenzophenone.* ***Hydrocotoin***

$C_{15}H_{14}O_4$ M 258.273

Occurs in Coto rind. Light-yellow prisms or needles (EtOH). Mp 97-98°.

2,6-Di-Me ether: 4-Hydroxy-2,6-dimethoxybenzophenone

$C_{15}H_{14}O_4$ M 258.273

Mp 178-179°.

Tri-Me ether: [3770-80-7]. *2,4,6-Trimethoxybenzophenone.* ***Methylhydrocotoin***

$C_{16}H_{16}O_4$ M 272.300

Isol. from Coto rind and *Cascara sagrada*. Prisms or tablets (EtOH). Mp 113-115°.

Karrer, P., *Helv. Chim. Acta*, 1928, **11**, 789 (*struct*)

Phadke, R. *et al, J. Indian Chem. Soc.*, 1950, **27**, 349 (*synth*)

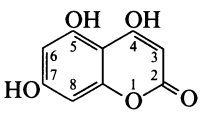
Gottleib, O.R. *et al, J. Am. Chem. Soc.*, 1958, **80**, 2263 (*isol, Cotoin*)

Harris, T.M. *et al, J. Am. Chem. Soc.*, 1966, **88**, 5686 (*synth*)

4,5,7-Trihydroxy-2H-1-benzopyran-2-one, 9CI **T-80286**

4,5,7-Trihydroxycoumarin

[17575-26-7]



$C_9H_6O_5$ M 194.143

Mp >300° dec. (sinters and browns from 210°).

Tri-Ac: Mp 155-156°.

Sonn, A., *Ber.*, 1917, **50**, 1292.

5,6,7-Trihydroxy-2*H*-1-benzopyran-2-one, 9CI — T-80287

Updated Entry replacing T-50456

5,6,7-Trihydroxycoumarin

$C_9H_6O_5$ M 194.143

7-Me ether: [50656-75-2]. *5,6-Dihydroxy-7-methoxy-2*H-1-*benzopyran-2-one, 9CI.* 5,6-*Dihydroxy-7-methoxycoumarin.* ***Isofraxetin***
$C_{10}H_8O_5$ M 208.170
Isol. from *Fraxinus potamophila* and *F. mandschurica*. Cryst. (MeOH). Mp 228-230°.

5,6-Di-Me ether: [43053-62-9]. *7-Hydroxy-5,6-dimethoxy-2*H-1-*benzopyran-2-one, 9CI.* 7-*Hydroxy-5,6-dimethoxycoumarin.* ***Umckalin***
$C_{11}H_{10}O_5$ M 222.197
Constit. of roots of *Pelargonium reniforme*. Mp 146-147°.

5,7-Di-Me ether: [486-28-2]. *6-Hydroxy-5,7-dimethoxy-2*H-1-*benzopyran-2-one, 9CI.* 6-*Hydroxy-5,7-dimethoxycoumarin.* ***Fraxinol***
$C_{11}H_{10}O_6$ M 238.196
Constit. of bark of *Fraxinus excelsior*. Exhibits spasmolytic activity. Mp 171-172°.

5,7-Di-Me ether, 6-O-glucoside: [32451-87-9]. ***Mandshurin.*** *Fraxinoside*
$C_{11}H_{10}O_5$ M 222.197
Constit. of bark of *F. potamophila* and *F. mandshurica*. Mp 134-136°, Mp 182.5°. $[\alpha]_D$ −26.7° (MeOH).

6,7-Di-Me ether: [28449-62-9]. *5-Hydroxy-6,7-dimethoxy-2*H-1-*benzopyran-2-one, 9CI.* 5-*Hydroxy-6,7-dimethoxycoumarin. Tomentin*
$C_{11}H_{10}O_5$ M 222.197
Aglycone from Tomenin. Cryst. (MeOH aq.). Mp 184-185°.

6,7-Di-Me ether, 5-glucoside: [28446-08-4]. ***Tomenin***
$C_{17}H_{20}O_{10}$ M 384.339
Constit. of *Prunus tomentosa*. Cryst. (MeOH). Mp 206°.

Tri-Me ether: [55085-47-7]. *5,6,7-Trimethoxy-2*H-1-*benzopyran-2-one, 9CI.* 5,6,7-*Trimethoxycoumarin*
$C_{12}H_{12}O_5$ M 236.224
Isol. from *P. reniforme*. Mp 74-75°.

Fujita, M. *et al, Chem. Pharm. Bull.*, 1958, **6**, 511 (*isol, Fraxinol*)
Artem'eva, M.V. *et al, Khim. Prir. Soedin.*, 1973, **9**, 493 (*isol*)
Wagner, H. *et al; Tetrahedron Lett.*, 1974, 3807 (*Umckalin, trimethoxycoumarin*)
Wagner, H. *et al, Phytochemistry*, 1975, **14**, 2061 (*Umckalin, trimethoxycoumarin*)
Murray, R.D.H. *et al, Tetrahedron*, 1975, **31**, 2966 (*struct*)
Ahluwalia, V.K. *et al, Indian J. Chem., Sect. B*, 1978, **16**, 591 (*synth*)

5,7,8-Trihydroxy-2*H*-1-benzopyran-2-one, 9CI — T-80288

5,7,8-Trihydroxycoumarin

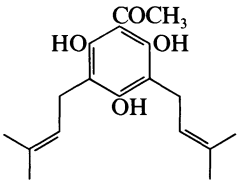
$C_9H_6O_5$ M 194.143

5,7-Di-Me ether: [61899-44-3]. *8-Hydroxy-5,7-dimethoxy-2*H-1-*benzopyran-2-one.* 8-*Hydroxy-5,7-dimethoxycoumarin.* ***Leptodactylone***
$C_{11}H_{10}O_5$ M 222.197
Isol. from *Ruta* spp., *Leptodactylon* spp. and *Lianthus* spp. Mp 149-152°, Mp 197-199°.

Tri-Me ether: [60796-65-8]. *5,7,8-Trimethoxy-2*H-1-*benzopyran-2-one.* 5,7,8-*Trimethoxycoumarin*
$C_{12}H_{12}O_5$ M 236.224
Isol. from *R.* spp. and *Toddalia aculeatra*. Mp 179-180° (165°).

Bandopadhyay, M. *et al, Indian J. Chem.*, 1974, **12**, 23 (*synth, uv*)
González, A.G. *et al, An. Quim.*, 1976, **72**, 191 (*isol*)
Deshmukh, M.N. *et al, Phytochemistry*, 1976, **15**, 1419 (*isol*)
Dan, F.M. *et al, Phytochemistry*, 1978, **17**, 505 (*isol*)

2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)acetophenone — T-80289



$C_{18}H_{24}O_4$ M 304.385

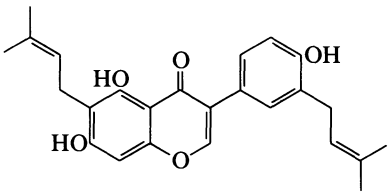
2-Me ether: 2,4-Dihydroxy-6-methoxy-3,5-bis(3-methyl-2-butenyl)acetophenone. 2,4-Dihydroxy-6-methoxy-3,5-diprenylacetophenone
$C_{19}H_{26}O_4$ M 318.412
Constit. of *Acronychia pedunculata*. Yellow oil.

Kumar, V. *et al, Phytochemistry*, 1989, **28**, 1278.

4′,5,7-Trihydroxy-3′,6-bis(3-methyl-2-butenyl)isoflavone — T-80290

*5,7-Dihydroxy-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-6-(3-methyl-2-butenyl)-4*H-*1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-3′,6-diprenylisoflavone. 3′-(γ,γ-Dimethylallyl)wighteone*

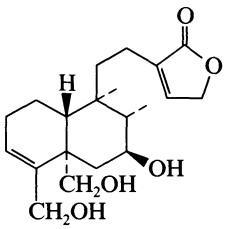
[76754-24-0]



$C_{25}H_{26}O_5$ M 406.477
Isol. from aerial parts of *Millettia pachycarpa*. Cryst. (C_6H_6/pet. ether). Mp 120°.

Singhal, A.K. *et al, Phytochemistry*, 1980, **19**, 929 (*isol, ir, uv, ms, struct*)

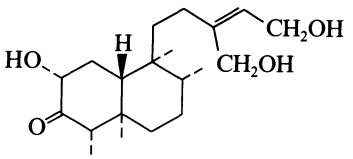
ent-7α,18,19-Trihydroxy-3,13-clerodadien-16,15-olide — T-80291



$C_{20}H_{30}O_5$ M 350.454
Constit. of *Salvia melissodora*. Cryst. (CH_2Cl_2/diisopropyl ether). Mp 149-150°. $[\alpha]_D^{20}$ −53.75° (c, 0.16 in $CHCl_3$).

Esquivel, B. *et al, Phytochemistry*, 1989, **28**, 561.

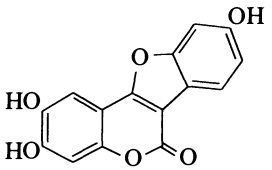
ent-2β,15,16-Trihydroxy-13-cleroden-3-one T-80292



$C_{20}H_{34}O_4$ M 338.486
Constit. of *Baccharis boliviensis*.
Tri-Ac: Oil. $[\alpha]_D^{24}$ +32° (c, 0.31 in $CHCl_3$).
Zdero, C. *et al*, *Phytochemistry*, 1989, **28**, 531.

2,3,9-Trihydroxycoumestan T-80293

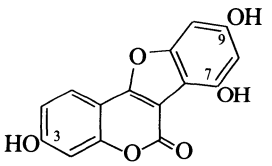
Updated Entry replacing L-00454
*2,3,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 9CI. **Lucernol.** 6,7,12-Trihydroxycoumestan*
[15402-22-9]



$C_{15}H_8O_6$ M 284.225
Constit. of alfalfa (*Medicago sativa*). Cryst. (DMSO). Mp >350°. λ_{max} 232, 310, 355 and 372 sh nm.
Tri-Me ether: Cryst. (MeOH). Mp 255°.
Spencer, R.R. *et al*, *J. Agric. Food Chem.*, 1966, **14**, 162 (*isol, struct*)
Kalna, V.K. *et al*, *Tetrahedron Lett.*, 1967, 2153 (*synth*)

3,7,9-Trihydroxycoumestan T-80294

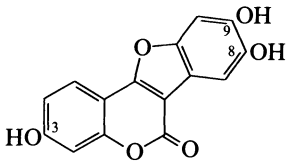
Updated Entry replacing W-20001
*3,7,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 9CI. 7,10,12-Trihydroxycoumestan. **Repensol***
[33280-69-2]



$C_{15}H_8O_6$ M 284.225
Isol. from fungus-infected *Trifolium repens* leaves. Cream needles (MeOH) (synthetic). Mp 346-348°.
9-Me ether: [1857-26-7]. *3,7-Dihydroxy-9-methoxycoumestan. **Trifoliol.** 7,10-Dihydroxy-12-methoxycoumestan*
$C_{16}H_{10}O_6$ M 298.251
Isol. from *T. repens* and *Medicago sativa*. Rods (DMF). Mp 332° dec.
7,9-Di-Me ether: [77331-73-8]. *3-Hydroxy-7,9-dimethoxycoumestan. **Wairol.** 7-Hydroxy-10,12-dimethoxycoumestan*
$C_{17}H_{12}O_6$ M 312.278
Isol. from *M. sativa*. Phytoalexin. Plates. Mp 292-294°.
Tri-Me ether: Cryst. (DMF). Mp 255-258°.
Bickoff, E.M. *et al*, *J. Pharm. Sci.*, 1964, **53**, 1496 (*isol*)
Livingston, A.L. *et al*, *Tetrahedron*, 1964, **20**, 1963 (*isol, struct, uv, synth*)
Wong, E. *et al*, *Phytochemistry*, 1971, **10**, 466 (*Repensol*)
Shaw, G.J. *et al*, *Phytochemistry*, 1980, **19**, 2801; 1982, **21**, 249 (*isol, synth*)

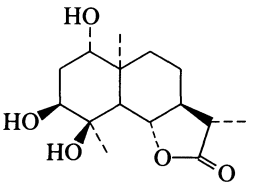
3,8,9-Trihydroxycoumestan T-80295

*3,8,9-Trihydroxy-6*H*-benzofuro[3,2-*c*]benzopyran-6-one, 9CI*



$C_{15}H_8O_6$ M 284.225
8-Me ether: 3,8-Dihydroxy-9-methoxycoumestan. 8-Methoxycoumestrol. 3′-Methoxycoumestrol (obsol.)
$C_{16}H_{10}O_6$ M 298.251
Isol. from *Medicago* spp. (alfalfa). Straw-coloured solid. Mp 329-329.5°.
8-Me ether, di-Ac: Needles. Mp 282-283°.
8,9-Di-Me ether: 3-Hydroxy-8,9-dimethoxycoumestan. 7-Hydroxy-11,12-dimethoxycoumestan (obsol.)
$C_{17}H_{12}O_6$ M 312.278
Isol. from *M. sativa* and *Myroxylon balsamum*. Solid (EtOAc). Mp 303-305°.
Bickoff, E.M. *et al*, *J. Agric. Food Chem.*, 1966, **14**, 444 (*isol*)
Spencer, R.R. *et al*, *J. Org. Chem.*, 1966, **31**, 988 (*isol, synth*)

1,3,4-Trihydroxy-12,6-eudesmanolide T-80296



$C_{15}H_{24}O_5$ M 284.352
(1α,3β,4β,6α,11βH,10α)-form [120163-09-9]
Constit. of *Pyrethrum santalinoides*. Gum. $[\alpha]_D^{24}$ +10° (c, 0.33 in $CHCl_3$).
Abdel-Mogib, M. *et al*, *Phytochemistry*, 1989, **28**, 268.

4′,5,8-Trihydroxyflavanone T-80297

[123067-25-4]
$C_{15}H_{12}O_5$ M 272.257
Constit. of *Artemisia campestris* ssp. *maritima*. Cryst. (MeOH aq.). Mp 262-264°.
Rauter, A.P. *et al*, *Phytochemistry*, 1989, **28**, 2173 (*isol, pmr*)

2′,5,5′-Trihydroxyflavone T-80298

[120552-44-5]
$C_{15}H_{10}O_5$ M 270.241
Constit. of *Primula pulverulenta*. Yellow powder. Mp >270° dec.
Wollenweber, E. *et al*, *Phytochemistry*, 1989, **28**, 295.

2′,5,7-Trihydroxyflavone T-80299

Updated Entry replacing D-04594
*5,7-Dihydroxy-2-(2-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*
$C_{16}H_{12}O_5$ M 284.268
7-Me ether: [4308-56-9]. *2′,5-Dihydroxy-7-methoxyflavone. **Echioidinin***
$C_{17}H_{14}O_5$ M 298.295
Constit. of *Andrographis echioides* and *A. wightiana*. Greenish-yellow needles (EtOH). Mp 264-266° dec.

7-Me ether, 2′-O-β-D-Glucopyranoside: ***Echioidin***
$C_{22}H_{22}O_{10}$ M 446.410
Isol. from *A. echioides*. Needles (Py/MeOH). Mp 276-278° dec. $[\alpha]_D^{24}$ −23.5° (c, 0.213 in Py/MeOH 1:1).

7-Me ether, di-Ac: Prisms (EtOAc). Mp 174-176°.

Govindachari, T.R. *et al*, *Tetrahedron*, 1965, **21**, 2633, 3715 (*isol, uv, ir, pmr, struct, synth*)
Farkas, L. *et al*, *Tetrahedron*, 1967, **23**, 741 (*synth*)

3,4′,7-Trihydroxyflavone T-80300

3,7-Dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. 4′,7-Dihydroxyflavonol

[2034-65-3]

$C_{15}H_{10}O_5$ M 270.241
Isol. from *Schinopsis lorentzii, Cicer arietinum, Rhus succedanea* and others. Light-yellow needles (EtOH or AcOH aq.). Mp 310° (304-306°).

Kirby, K.S. *et al*, *Biochem. J.*, 1955, **60**, 582 (*isol, struct, synth*)
Wong, E. *et al*, *Phytochemistry*, 1965, **4**, 89 (*isol, synth*)
Hillis, W.E. *et al*, *Phytochemistry*, 1966, **5**, 483 (*isol*)

3′,4′,7-Trihydroxyflavone T-80301

$C_{15}H_{10}O_5$ M 270.241

$O^{3'}$*-Me:* [21583-32-4]. *4′,7-Dihydroxy-3′-methoxyflavone.* ***Geraldone***
$C_{16}H_{12}O_5$ M 284.268
Isol. from subterranean clover *Trifolium subterraneum*. Minute off-white cryst. Mp 293-294° dec.

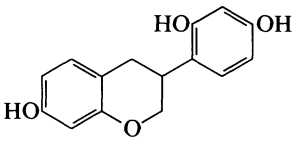
$O^{3'}$*-Me, 7-glucoside:*
$C_{22}H_{22}O_{10}$ M 446.410
Isol. from *T. subterraneum*.

Wong, E. *et al*, *Phytochemistry*, 1968, **7**, 2123 (*isol, struct, synth*)

2′,4′,7-Trihydroxyisoflavan T-80302

4-(3,4-Dihydro-7-hydroxy-2H-1-benzopyran-4-yl)-1,3-benzenediol, 9CI. 3,4-Dihydro-3-(2,4-dihydroxyphenyl)-7-hydroxy-2H-1-benzopyran. ***Demethylvestitol***

[65332-45-8]



$C_{15}H_{14}O_4$ M 258.273
Compds. in both enantiomeric series appear to occur naturally but in most cases the abs. config.was not detd.
Isol. from *Anthyllis vulneraria, Erythrina sandwicensis, Hosackia americana, Lablab niger, Lotus* spp., *Phaseolus vulgaris* and *Tetragonolobus* spp.

2′-Me ether: [63631-42-5]. *4′,7-Dihydroxy-2′-methoxyisoflavan.* ***Isovestitol***
$C_{16}H_{16}O_4$ M 272.300
Constit. of *A. vulneraria, E. sandwicensis, H. americana, Lablab niger, T.* spp. and *Trifolium* spp.

7-Me ether: [71772-21-9]. *2′,4′-Dihydroxy-7-methoxyisoflavan.* ***Neovestitol***
$C_{16}H_{16}O_4$ M 272.300
Isol. from leaves of *Dalbergia sericea*.

2′,4′-Di-Me ether: [41743-86-6]. *7-Hydroxy-2′,4′-dimethoxyisoflavan.* ***Sativan.*** *Sativin. 2′-O-Methylvestitol*
$C_{17}H_{18}O_4$ M 286.327
Isol. from *Derris amazonica, Lotus* spp., *Medicago* spp., *Trifolium* spp. and *Trigonella* spp. Cryst. Mp 128-129° (125-127°). $[\alpha]_D^{22}$ −15°. Mp. refers to the (*S*)-enantiomer from *D. amazonica*.

2′,7-Di-Me ether: [63631-41-4]. *4′-Hydroxy-2′,7-dimethoxyisoflavan.* ***Arvensan***
$C_{17}H_{18}O_4$ M 286.327
Stress metab. from *Trifolium arvense* and *T. stellatum*. Mp 111-115°.

4′,7-Di-Me ether: [60102-29-6]. *2′-Hydroxy-4′,7-dimethoxyisoflavan.* ***Isosativan***
$C_{17}H_{18}O_4$ M 286.327
Isol. from *Dalbergium ecastophyllum, M. scutellata, M. rugosa* and *Trifolium* spp.

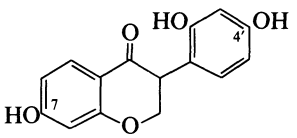
[64190-84-7, 75556-92-2]

Ingham, J.L. *et al*, *Nature* (*London*), 1973, **242**, 125 (*Sativan*)
Braz Filho, R. *et al*, *Phytochemistry*, 1975, **14**, 1454 (*isol*)
Ingham, J.L., *Z. Naturforsch., C*, 1976, **31**, 331; 1977, **32**, 446,1018; 1979, **34**, 630; 1980, **35**, 384.
Ingham, J.L. *et al*, *Phytochemistry*, 1977, **16**, 1279; 1979, **18**, 1711 (*isol, struct*)
Alves, H.M. *et al*, *Phytochemistry*, 1978, **17**, 1423 (*synth*)
Ingham, J.L. *et al*, *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

2′,4′,7-Trihydroxyisoflavanone T-80303

Updated Entry replacing T-20259

2,3-Dihydro-7-hydroxy-3-(2,4-dihydroxyphenyl)-4H-1-benzopyran-4-one. 2′-Hydroxydihydrodaidzein



$C_{15}H_{12}O_5$ M 272.257

(±)***-form***
Isol. from pods of *Phaseolus vulgaris*.

4′-Me ether: [57462-46-1]. *2′,7-Dihydroxy-4′-methoxyisoflavanone.* ***Vestitone***
$C_{16}H_{14}O_5$ M 286.284
Isol. from *Medicago rugosa, Onobrychis vicifolia, Tipuana tipu* and *Trifolium repens*.

2′,4′-Di-Me ether: [70561-31-8]. *7-Hydroxy-2′,4′-dimethoxyisoflavanone.* ***Sativanone***
$C_{17}H_{16}O_5$ M 300.310
Isol. from heartwood of *Dalbergia stevensonii* and leaves of *M. sativa*. Needles (C_6H_6/pet. ether). Mp 184-185°.

4′,7-Di-Me ether: [82829-55-8]. *2′-Hydroxy-4′,7-dimethoxyisoflavanone.* ***Isosativanone***
$C_{17}H_{16}O_5$ M 300.310
Constit. of *M. rugosa*.

Donnelly, D.M.X. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1973, 1737 (*Sativanone*)
Derrick, P.M., *Phytochemistry*, 1977, **16**, 93 (*Vestitone*)
Ingham, J.L., *Z. Naturforsch., C*, 1978, **33**, 146 (*Vestitone*)
Woodward, M.D., *Phytochemistry*, 1980, **19**, 921 (*isol, uv, pmr*)
Ingham, J.L., *Planta Med.*, 1982, **45**, 46 (*isol*)
Jain, A.C. *et al*, *Indian J. Chem., Sect. B*, 1987, **26**, 136 (*synth*)

4′,5,7-Trihydroxyisoflavanone T-80304

2,3-Dihydro-5,7-dihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one

$C_{15}H_{12}O_5$ M 272.257

(*S*)***-form***
5,7-*Dihydroxy-4′-methoxyisoflavanone.* ***Dihydrobiochanin A***

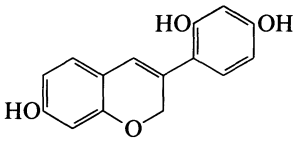
$C_{16}H_{14}O_5$ M 286.284
Isol. from *Andira parviflora* trunkwood. Mp 167-169°.

Braz Filho, R. *et al*, *Phytochemistry*, 1973, **12**, 1184 (*isol, ir, ms, pmr, struct*)

2′,4′,7-Trihydroxyisoflavene T-80305

*4-(7-Hydroxy-2*H*-1-benzopyran-3-yl)-1,3-benzenediol, 9CI.* ***Haginin D***

[79852-13-4]



$C_{15}H_{12}O_4$ M 256.257
Isol. from heartwood of *Lespedeza cyrtobotrya*. Prisms (Me_2CO/hexane). Mp 192-195° dec.

2′-Me ether: [74174-31-5]. *4′,7-Dihydroxy-2′-methoxyisoflavene.* 3-(4-*Hydroxy-2-methoxyphenyl*)-2H-1-*benzopyran-7-ol, 9CI.* ***Haginin B***
$C_{16}H_{14}O_4$ M 270.284
Isol. from heartwood of *L. cyrtobotrya*.

2′-Me ether, di-Ac: Needles ($CHCl_3$/MeOH). Mp 128-129°.

Miyase, T. *et al*, *Chem. Pharm. Bull.*, 1980, **28**, 1172; 1981, **29**, 2205 (*isol, uv, pmr, struct*)

2′,4′,7-Trihydroxyisoflavone T-80306

*3-(2,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI. 2′-Hydroxydaidzein*

[7678-85-5]

$C_{15}H_{10}O_5$ M 270.241
Isol. from pods of *Phaseolus vulgaris*. Cryst. (MeOH). Mp 275° dec. (synthetic).

2′-Me ether: [56581-76-1]. *4′,7-Dihydroxy-2′-methoxyisoflavone.* ***Teralin.*** *Theralin*
$C_{16}H_{12}O_5$ M 284.268
Isol. from leaves of *Thermopsis alterniflora*. Dark-yellow cryst. (MeOH). Mp 275°.

4′-Me ether: [1890-99-9]. *2′,7-Dihydroxy-4′-methoxyisoflavone. 2′-Hydroxyformononetin*
$C_{16}H_{12}O_5$ M 284.268
Isol. from *Trifolium repens, Virola caducifolia* and *V. multinervia*. Cryst. ($CHCl_3$/MeOH). Mp 215-217°.

Kattaev, N.S. *et al*, *Khim. Prir. Soedin.*, 1975, 140; *cnc*, 157 (*Teralin*)
Braz Filho, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1977, **40**, 236 (2′,7-Dihydroxy-4′-methoxyisoflavone)
Woodward, M.D., *Phytochemistry*, 1980, **19**, 921 (*isol, uv, pmr, ms, struct*)

2′,5,7-Trihydroxyisoflavone T-80307

Isogenistein

[70943-68-9]

$C_{15}H_{10}O_5$ M 270.241
Long straw-yellow needles (MeOH). Mp 222-224° (sinters at 190°).

7-O-Glucoside: [70943-69-0].
$C_{21}H_{20}O_{10}$
Isol. from rootbark of *Cajanus cajan*. Needles (EtOH). Mp 200-203°.

Bhanumati, S. *et al*, *Phytochemistry*, 1979, **18**, 365.

3′,4′,7-Trihydroxyisoflavone T-80308

Updated Entry replacing D-04601

*3-(3,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′-Hydroxydaidzein*

$C_{15}H_{10}O_5$ M 270.241
Isol. from heartwood of *Machaerium villosum*. Mp 252° (245-250°) (synthetic).

3′-Me ether: [21913-98-4]. *4′,7-Dihydroxy-3′-methoxyisoflavone. 3′-Methoxydaidzein*
$C_{16}H_{12}O_5$ M 284.268
Isol. from *Cyclobium clausseni, Maackia amurensis* and *Machaerium villosum*. Plates (MeOH). Mp 262°.

4′-Me ether: [20575-57-9]. *3′,7-Dihydroxy-4′-methoxyisoflavone.* ***Calycosin***
$C_{16}H_{12}O_5$ M 284.268
Isol. from *Baptisia, Bowdichia, Cadia, Cladrastis, Cyclobium, Dalbergia, Machaerium, Myroxylon, Pterocarpus, Sophora, Thermopsis* and *Trifolium* spp. (all Leguminosae subfamily Paplilionoideae). Cryst. (EtOH). Mp 245-247° (228-230°).

4′-Me ether, 7-O-glucoside: [20633-67-4].
$C_{22}H_{22}O_{10}$ M 446.410
Isol. from *Baptisia* and *Thermopsis* spp. λ_{max} 255, 327 nm (MeOH).

4′-Me ether, 7-O-rhamnosylglucoside:
$C_{28}H_{32}O_{15}$ M 608.552
Isol. from *B.* spp.

3′,4′-Di-Me ether: [24160-14-3]. *7-Hydroxy-3′,4′-dimethoxyisoflavone.* ***Cladrin***
$C_{17}H_{14}O_5$ M 298.295
Constit. of *Cladrastis lutea* heartwood. Mp 257-258°.

3′,7-Di-Me ether: [30564-92-2]. *4′-Hydroxy-3′,7-dimethoxyflavone.* ***Sayanedine***
$C_{17}H_{14}O_5$ M 298.295
Isol. from pods of *Pisum sativum*. Needles (hexane). Mp 165-166°.

Tri-Me ether: 3′,4′,7-Trimethoxyisoflavone. ***Cabreuvin***
$C_{18}H_{16}O_5$ M 312.321
Isol. from *Calopogonium mucunoides, Myrocarpus fastigiatus*, and *Myroxylon* spp. Mp 156-158°.

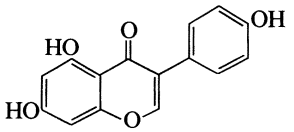
Gottlieb, O.R. *et al*, *An. Assoc. Quim. Bras.*, 1959, **18**, 85 (*Cabreuvin*)
Fukui, F. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1963, **84**, 189 (*synth*)
Braga de Oliveira, A. *et al*, *Ann. Acad. Bras. Cienc.*, 1968, **40**, 147 (*isol*)
Markham, K.R. *et al*, *Phytochemistry*, 1968, **7**, 803 (*glycosides*)
Shamma, M. *et al*, *Tetrahedron*, 1969, **25**, 3887 (*Cladrin*)
Isogai, Y. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 1872 (*Sayanedine*)
Farkas, L. *et al*, *Acta Chim. Acad. Sci. Hung.*, 1972, **74**, 367 (*synth*)
Takai, M. *et al*, *Chem. Pharm. Bull.*, 1972, **20**, 2488 (*4′,7-Dihydroxy-3′-methoxyisoflavone, synth*)
Brown, P.M. *et al*, *Justus Liebigs Ann. Chem.*, 1974, 1295 (*Calycosin*)
Dewick, P.M. *et al*, *Phytochemistry*, 1978, **77**, 1751 (*biosynth*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

4′,5,7-Trihydroxyisoflavone T-80309

Updated Entry replacing T-60324

*5,7-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Genistein.*** *Differenol A. Prunetol. Sophoricol*

[446-72-0]



$C_{15}H_{10}O_5$ M 270.241

V. widely distributed in the Leguminosae subf. Papilionoideae but also in *Podocarpus spicatus* (Podocarpaceae) and *Prunus* spp. (Rosaceae). Also prod. by microorganisms *Streptomyces* spp., *Aspergillus niger*, *Mycobacterium phlei* and *Micromonospora haplophytica*. Weak oestrogen. Shows insect antifeedant and weak antibacterial activity against *E. coli* and *Xanthomonas oryzae*. Induces cell differentiation and inhibits DOPA carboxylase. Prisms (EtOH aq.). Mp 301-302° dec. Methylgenistein, Isogenistin and Methylisogenistin were all impure Genistein.

▷ Exp. carcinogen. NR2392000.

4-β-D-Glucoside: [152-95-4]. ***Sophoricoside***
$C_{21}H_{20}O_{10}$ M 432.383
Constit. of *Sophora japonica* and *Piptanthus nepalensis*. Prisms (EtOH). Mp 297°. $[\alpha]_D^{20}$ −46.7°.

7-β-D-Glucoside: [529-59-9]. ***Genistin.*** *Genistoside*
$C_{21}H_{20}O_{10}$ M 432.383
Isol. from *Genista* spp., *Lupinus* spp. and a number of other spp. in the Leguminosae subfamily Papilionoideae. Also in *Prunus aequinoctalis*, *P. avium* and *P. nipponica* (Rosaceae). Leaflets (EtOH). Mp 254-256° dec. $[\alpha]_D^{21}$ −27.7° (MeOH aq.).

7-β-D-Rutinoside: [14988-20-6]. ***Sphaerobioside***
$C_{27}H_{30}O_{14}$ M 578.526
Isol. from *Baptisia sphaerocarpa* and *B. lecontii*. Needles (MeOH). Mp 203-204°. $[\alpha]_D^{20}$ −73.3° (c, 9.9 in Py).

4′,7-Bis(4-O-β-D-glucopyranosyl-β-D-apiofuranoside): [78693-95-5]. ***Sarothamnoside***
$C_{37}H_{46}O_{23}$ M 858.757
Obt. from seeds of *Sarothamnus* spp. Mp 136-138°. $[\alpha]_D^{20}$ −128° (c, 0.1 in H_2O).

7-O-[Apiosyl-(1→6)-β-D-glucopyranoside]: [108044-05-9]. ***Ambocin***
$C_{26}H_{28}O_{14}$ M 564.499
Constit. of *Neorautanenia amboensis*. Glass. $[\alpha]_D$ −36.5° (c, 0.011 in H_2O).

4′-Apioside, 7-β-D-glucopyranoside: [108069-00-7]. ***Neobacin***
$C_{26}H_{28}O_{14}$ M 564.499
From *N. amboensis*. Glass. $[\alpha]_D$ −38.2° (c, 0.011 in H_2O).

7-O-Glucosylglucoside:
$C_{27}H_{30}O_{15}$ M 594.525
Isol. from *Lupinus angustifolius*, *L. polyphyllus and L. luteus*.

4′,7-Di-O-glucoside:
$C_{27}H_{30}O_{15}$ M 594.525
Isol. from *Piptanthus nepalensis* and *Thermopsis* spp.

7-O-(6-O-Acetyl-β-D-glucopyranoside): [72741-92-5]. ***6″-O-Acetylgenistin***
$C_{23}H_{22}O_{11}$ M 474.420
Isol. from seeds of *Glycine max* (soybean). Needes. Mp 185-186°.

4′-O-Neohesperidoside: [2945-88-2]. ***Sophorabioside***
$C_{27}H_{30}O_{14}$ M 578.526
Isol. from *Sophora japonica*. Yellowish needles + $3H_2O$. Mp 245-248° (unsharp)(anhyd.). $[\alpha]_D^{19}$ −72.5° (Py)(anhyd.).

7-O-(6-O-Malonyl-D-glucoside): ***Genistein 7-O-glucoside 6″-malonate***
$C_{24}H_{22}O_{13}$ M 518.430
Isol. from leaves of *Trifolium subterraneum*. Poss. accompanied by its Me ester. Glass. Mp 160° approx.

4′-Me ether: see *5,7-Dihydroxy-4′-methoxyisoflavone*, D-80337

7-Me ether: see *4′,5-Dihydroxy-7-methoxyisoflavone*, D-80335

4′,5-Di-Me ether: [68939-22-0]. *7-Hydroxy-4′,5-dimethoxyisoflavone*. 5-O-*Methylbiochanin A*
$C_{17}H_{14}O_5$ M 298.295
Isol. from *Echinospartum horridum* (after hydrol.) and cultures of *Fusarium* spp. Mp 294-296°.

Bognár, R. *et al*, *Chem. Ind.* (*London*), 1954, 518 (*Sophoricoside, synth*)
Rosler, H. *et al*, *Chem. Ber.*, 1965, **98**, 2193 (*deriv*)
Wagner, H. *et al*, *Chem. Ber.*, 1967, **100**, 101 (*synth*)
Farkas, L. *et al*, *Chem. Ber.*, 1968, **101**, 2758 (*Sophorabioside*)
Markham, K.R. *et al*, *Phytochemistry*, 1968, **7**, 791 (*isol*)
Ganguly, A.K. *et al*, *Chem. Ind.* (*London*), 1970, 201 (*isol*)
Umezawa, H. *et al*, *J. Antibiot.*, 1975, **28**, 947 (*isol*)
Wagner, H. *et al*, *Tetrahedron Lett.*, 1976, 1799 (*cmr*)
Grayer-Barkmeijer, R.J. *et al*, *Phytochemistry*, 1978, **17**, 829 (*7-Hydroxy-4′,5-dimethoxyisoflavone*)
Hazeto, T. *et al*, *J. Antibiot.*, 1979, **32**, 217 (*isol*)
Ohta, N. *et al*, *Agric. Biol. Chem.*, 1980, **44**, 469 (6′-O-Acetylgenistin)
Asahi, K. *et al*, *J. Antibiot.*, 1981, **34**, 919 (*uv, ir*)
Brum-Bousquet, M. *et al*, *Tetrahedron Lett.*, 1981, 1223 (*Sarothamnoside*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Ogawara, H. *et al*, *J. Antibiot.*, 1986, **39**, 606 (*Ambocin, Neobacin*)
Jain, A.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1986, 215 (*synth*)
Breytenbach, J.C., *J. Nat. Prod.* (*Lloydia*), 1986, **49**, 1003 (*isol, deriv*)

4′,6,7-Trihydroxyisoflavone T-80310

Updated Entry replacing T-60325

[17817-31-1]

$C_{15}H_{10}O_5$ M 270.241

Isol. from fermented soybeans. Cryst. (MeOH). Mp 322°.

Tri-Ac: Cryst. (EtOH). Mp 217°.

6-Me ether: 4′,7-Dihydroxy-6-methoxyisoflavone. ***Glycitein***
$C_{16}H_{12}O_5$ M 284.268
Isol. from *Centrosema haitense*, *C. pubescens*, *Glycine max* and *Mildraeodendron excelsa*. Cryst. (MeOH). Mp 311-313°.

7-Me ether: [57960-04-0]. *4′,6-Dihydroxy-7-methoxyisoflavone.* ***Kakkatin***
$C_{16}H_{12}O_5$ M 284.268
Isol. from flowers of *Pueraria* spp. Needles (MeOH). Mp >290°.

4′,7-Di-Me ether: [550-79-8]. *6-Hydroxy-4′,7-dimethoxyisoflavone.* ***Afrormosin.*** *Afromosin. Castanin*
$C_{17}H_{14}O_5$ M 298.295
Constit. of *Afrormosia elata*, *Castanospermum australe* and *Myrocarpus* spp. and from other spp. in the Leguminosae (Papilionoideae). Needles (MeOH or EtOH). Mp 236-237° (228-229°).

4′,7-Di-Me ether, 6-β-D-glucopyranosyl: [19046-26-5]. ***Wistin***
$C_{23}H_{24}O_9$ M 444.437

Constit. of *Wistaria floribunda*. Needles (MeOH aq. or Me_2CO aq.). Mp 209-210°. $[\alpha]_D^{12}$ −67.15° (c, 1.43 in AcOH).

Tri-Me ether: [798-61-8]. *4′,6,7-Trimethoxyisoflavone*
$C_{18}H_{16}O_5$ M 312.321
Cryst. Mp 179-180°.

McMurry, T.B.H. *et al*, *J. Chem. Soc.*, 1960, 1491 (*isol, struct*)
Fujita, M. *et al*, *Chem. Pharm. Bull.*, 1963, **11**, 382 (*deriv*)
Harbourne, J. *et al*, *J. Org. Chem.*, 1963, **28**, 881 (*isol*)
Bevan, C.W.L. *et al*, *J. Chem. Soc. C*, 1966, 509 (*isol, struct*)
Ikehata, H. *et al*, *Agric. Biol. Chem.*, 1968, **32**, 740 (*isol*)
Birk, Y. *et al*, *Phytochemistry*, 1973, **12**, 169 (*Glycitein*)
Antus, S. *et al*, *Chem. Ber.*, 1975, **108**, 3883 (*synth, Glycitein*)
Kubo, M. *et al*, *Chem. Pharm. Bull.*, 1975, **23**, 2449 (*Kakkatin*)
Donnelly, D.M.X. *et al*, *Phytochemistry*, 1975, **14**, 2283 (*synth, Glycitein*)
Dewick, P.M. *et al*, *Phytochemistry*, 1978, **17**, 249 (*biosynth*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Caballero, P. *et al*, *J. Nat. Prod.* (*Lloydia*), 1986, **49**, 1126 (*cryst struct*)

4′,7,8-Trihydroxyisoflavone T-80311

Updated Entry replacing D-04604

*7,8-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one*
$C_{15}H_{10}O_5$ M 270.241

4′-Me ether: [37816-19-6]. *7,8-Dihydroxy-4′-methoxyisoflavone*. ***Retusin***
$C_{16}H_{12}O_5$ M 284.268
Isol. from heartwood of *Dalbergia retusa* and *Dipteryx odorata*. Cryst. (Me_2CO/MeOH or Me_2CO). Mp 249°.

4′,8-Di-Me ether: [37816-20-9]. *7-Hydroxy-4′,8-dimethoxyisoflavone*. 8-O-*Methylretusin*
$C_{17}H_{14}O_5$ M 298.295
Isol. from *Cladrastis* spp., *Dalbergia retusa*, *D. variabilis*, *Dipteryx odorata*, *Monopteryx uaucu*, *Pericopsis schliebenii* and *Xanthocercus zambesiaca* (all Leguminosae). Prisms (Me_2CO/MeOH). Mp 221°.

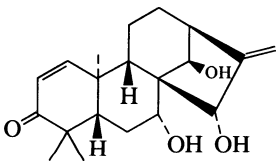
4′,8-Di-Me ether, 7-O-glucoside:
$C_{23}H_{24}O_{10}$ M 460.437
Isol. from *C. platycarpa*, *C. shikokiana* and *Wisteria floribunda* bark.

4′,8-Di-Me ether, 7-O-laminarabioside:
$C_{29}H_{34}O_{15}$ M 622.579
Isol. from *C. platycarpa* and *C. shikokiana*. Needles. Mp 194-195°.

Jurd, L. *et al*, *Phytochemistry*, 1972, **11**, 2535 (8-*O*-Methylretusin)
Jurd, L. *et al*, *Tetrahedron Lett.*, 1972, 2149 (*Retusin*)
Hayashi, T. *et al*, *Phytochemistry*, 1974, **13**, 1943 (*Retusin*)
Imamura, H. *et al*, *Phytochemistry*, 1974, **13**, 757 (*Glucoside*)
Farkas, L. *et al*, *Acta Chim. Acad. Sci. Hung.*, 1976, **88**, 173 (*synth*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)

ent-7β,14α,15β-Trihydroxy-1,16-kauradien-3-one T-80312

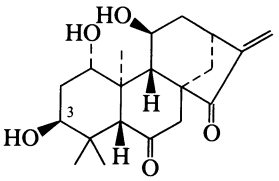
Liangshanin D



$C_{20}H_{28}O_4$ M 332.439
Constit. of *Rabdosia liangshanica*. Cryst. Mp 302-305°.

Fenglei, Z. *et al*, *Phytochemistry*, 1989, **28**, 1671.

ent-1β,3α,11α-Trihydroxy-16-kaurene-6,15-dione T-80313



$C_{20}H_{28}O_5$ M 348.438

3-Ac: ent-3α-*Acetoxy*-1β,11α-*dihydroxy*-16-*kaurene*-6,15-*dione*. ***Inflexarabdonin E***
$C_{22}H_{30}O_6$ M 390.475
Constit. of *Rabdosia inflexa*. Cryst. Mp 234-237°. $[\alpha]_D$ −42.8° (c, 0.8 in MeOH).

Takeda, Y. *et al*, *Phytochemistry*, 1989, **28**, 2423 (*isol, pmr, cmr*)

ent-1β,7β,14α-Trihydroxy-16-kaurene-3,15-dione T-80314

$C_{20}H_{28}O_5$ M 348.438

1-Ac: ent-1β-*Acetoxy*-7β,14α-*dihydroxy*-16-*kaurene*-3,15-*dione*. ***Liangshanin E***
$C_{22}H_{30}O_6$ M 390.475
Constit. of *Rabdosia liangshanica*. Cryst. Mp 138-140°.

Fenglei, Z. *et al*, *Phytochemistry*, 1989, **28**, 1671.

ent-7β,12β,14α-Trihydroxy-16-kaurene-3,15-dione T-80315

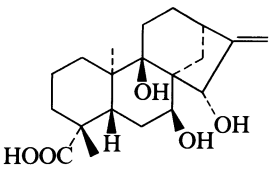
$C_{20}H_{28}O_5$ M 348.438

12-Ac: ent-12β-*Acetoxy*-7β,14α-*dihydroxy*-16-*kaurene*-3,15-*dione*. ***Liangshanin F***
$C_{22}H_{30}O_6$ M 390.475
Constit. of *Rabdosia liangshanica*. Cryst. Mp 220-222°.

Fenglei, Z. *et al*, *Phytochemistry*, 1989, **28**, 1671.

ent-7α,9α,15β-Trihydroxy-16-kauren-19-oic acid T-80316

[122585-73-3]



$C_{20}H_{30}O_5$ M 350.454
Constit. of *Helichrysum dasyanthum*.

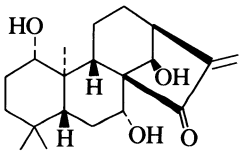
Jakupovic, J., *Phytochemistry*, 1989, **28**, 1119.

ent-1β,7β,14*S*-Trihydroxy-16-kauren-15-one T-80317

Updated Entry replacing T-50476

Kamebanin

[39388-57-3]



$C_{20}H_{30}O_4$ M 334.455

Constit. of *Isodon kameba*. Cryst. Mp 266-267°. $[\alpha]_D^{19}$ −108° (c, 1 in dioxan).

7-Ac: ent-7*β*-*Acetoxy*-1*β*,14S-*dihydroxy*-16-*kauren*-15-*one*
$C_{22}H_{32}O_5$ M 376.492
Constit. of *Rabdosia umbrosia*. Needles. Mp 201-202°. $[\alpha]_D^{22}$ −121.8° (c, 0.63 in MeOH).

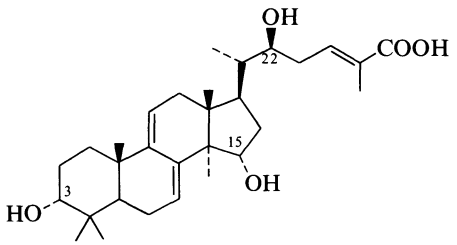
14-Ac: ent-14S-*Acetoxy*-1*β*,7*β*-*dihydroxy*-16-*kauren*-15-*one*
$C_{22}H_{32}O_5$ M 376.492
Constit. of *R. umbrosia*. Amorph. powder. $[\alpha]_D^{22}$ −94.0° (c, 0.47 in MeOH).

Tri-Ac: Needles. Mp 196-198°.

Kubo, I. *et al*, *Chem. Lett.*, 1977, 1289 (*isol, struct*)
Takeda, Y. *et al*, *Phytochemistry*, 1989, **28**, 1691 (*derivs*)

3,15,22-Trihydroxy-7,9(11),24-lanostatrien-26-oic acid T-80318

Updated Entry replacing T-70266



$C_{30}H_{46}O_5$ M 486.690
The Ganoderic/Ganodermic synonyms are best avoided as many of them have been duplicated. Use systematic names.

(3α,15α,22S,24E)-form

3-Ac: 3*α*-*Acetoxy*-15*α*,22S-*dihydroxy*-7,9(11),24E-*lanostatrien*-26-*oic acid*
$C_{32}H_{48}O_6$ M 528.728
Constit. of *Ganoderma lucidum*.

22-Ac: 22S-*Acetoxy*-3*α*,15*α*-*dihydroxy*-7,9(11),24-*lanostatren*-26-*oic acid*
$C_{32}H_{48}O_6$ M 528.728
Constit. of *G. lucidum*.

15,22-Di-Ac: [112667-14-8]. 15*α*,22S-*Diacetoxy*-3*α*-*hydroxy*-7,9(11),24E-*lanostatrien*-26-*oic acid. Ganoderic acid P*
$C_{34}H_{50}O_7$ M 570.765
Constit. of the cultured mycelium of *G. lucidum*. Cryst. Mp 211-212.5°.

3,22-Di-Ac: [110024-14-1]. 3*α*,22S-*Diacetoxy*-15*α*-*hydroxy*-7,9(11),24E-*lanostatrien*-26-*oic acid. Ganoderic acid Q. Ganodermic acid P*1
$C_{34}H_{50}O_7$ M 570.765
Constit. of the cultured mycelium of *G. lucidum*. Cryst. Mp 131-132°. Also descr. as a resin.

Tri-Ac: [103992-91-2]. 3*α*,15*α*,22S-*Triacetoxy*-7,9(11),24-*lanostatrien*-26-*oic acid. Ganoderic acid T*
$C_{36}H_{52}O_8$ M 612.802
Constit. of cultured mycelium of *G. lucidum*. Cryst. Mp 200-202°. $[\alpha]_D$ +23° (c, 0.13 in $CHCl_3$).

(3α,15α,22ξ,24E)-form

3,22-Di-Ac: 3*α*,22*ξ*-*Diacetoxy*-15*α*-*hydroxy*-7,9(11),24-*lanostatrien*-26-*oic acid. Ganoderic acid Mk*
$C_{34}H_{50}O_7$ M 570.765
Constit. of *G. lucidum*. Syrup. $[\alpha]_D^{23}$ +23° (c, 0.2 in MeOH). Not clear whether this is identical with Ganoderic acid Q above.

(3β,15α,22S,24E)-form

Constit. of *G.lucidum*. Needles ($CHCl_3$/MeOH). Mp 178-180°.

15,22-Di-Ac: [112430-69-0]. 15*α*,22S-*Diacetoxy*-3*β*-*hydroxy*-7,9(11),24E-*lanostatrien*-26-*oic acid. Gandodermic acid P*2
$C_{34}H_{50}O_7$ M 570.765
Metab. of *G. lucidum*. Resin.

Tri-Ac: [112430-70-3]. 3*β*,15*α*,22S-*Triacetoxy*-7,9(11),24E-*lanostatrien*-26-*oic acid*
$C_{36}H_{52}O_8$ M 612.802
Metab. of *G. lucidum*.

22-Ac: 22S-*Acetoxy*-3*β*,15*α*-*dihydroxy*-7,9(11),24-*lanostatrien*-26-*oic acid*
$C_{32}H_{48}O_6$ M 528.728
Constit. of *G. lucidum*.

(3α,15α,22R,24E)-form

Constit. of *G. lucidum*.

3,15-Di-Ac: 3*α*,15*α*-*Diacetoxy*-22R-*hydroxy*-7,9(11),24-*lanostatrien*-26-*oic acid*
$C_{34}H_{50}O_7$ M 570.765
Constit. of *G. lucidum*.

(3β,15α,22R,24E)-form

3,15-Di-Ac: 3*β*,15*α*-*Diacetoxy*-22R-*hydroxy*-7,9(11)24-*lanostatrien*-26-*oic acid*
$C_{34}H_{50}O_7$ M 570.765
Constit. of *G. lucidum*.

Toth, J.O. *et al*, *Tetrahedron Lett.*, 1983, **24**, 1081 (*isol, deriv*)
Hirotani, M. *et al*, *Chem. Pharm. Bull.*, 1986, **34**, 2282 (*isol*)
Nishitoba, T. *et al*, *Agric. Biol. Chem.*, 1987, **51**, 1149 (*isol*)
Hirotani, M. *et al*, *Phytochemistry*, 1987, **26**, 2797 (*isol*)
Lin, L.-J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 918 (*isol*)
Shiao, M.-S. *et al*, *Phytochemistry*, 1988, **27**, 873, 2911 (*isol*)

4′,5,7-Trihydroxy-6-methoxyisoflavone T-80319

Updated Entry replacing T-20263

*5,7-Dihydroxy-3-(4-hydroxyphenyl)-6-methoxy-4*H*-1-benzopyran-4-one, 9CI.* ***Tectorigenin***

[548-77-6]

$C_{16}H_{12}O_6$ M 300.267
Isol. from *Baptisia* spp., *Centrosema* spp., *Dalbergia* spp. and *Ononis spinosa* (all Leguminosae, Papilionoideae) and also *Iris germanica*. Yellow plates (EtOH) or needles (C_6H_6/EtOH). Mp 235-237° (227° dec.).

▷ NR2400000.

7-O-β-D-Glucopyranoside: [611-40-5]. ***Tectoridin.*** *Shekanin*
$C_{18}H_{22}O_{11}$ M 414.365
Isol. from *Baptisia* spp., *Belamcanda chinensis*, *Dalbergia* spp., *Iris* spp. and *Pueraria montana*. Needles. Mp 257° dec. $[\alpha]_D^{20}$ −29.4° (Py).

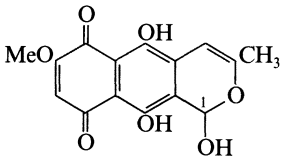
7-O-Gentobioside: [67604-94-8].
$C_{28}H_{32}O_{16}$ M 624.551
Isol. from bark of *Dalbergia volubilis*. Mp 160-162°. $[\alpha]_D$ −37.2° (c, 0.65 in MeOH).

4′-O-(3-Methyl-2-butenyl): [87457-87-2]. ***Isoaurmillone***
$C_{21}H_{20}O_6$ M 368.385
Constit. of pods of *Millettia auriculata*. Yellow needles ($CHCl_3$/pet. ether). Mp 162.5-163.5°.

Mannich, C. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1937, **275**, 317 (*Tectoridin*)
Shriner, R.L. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 2737 (*struct, synth*)
Várady, J., *Tetrahedron Lett.*, 1965, 4273 (*synth*)
Baker, W. *et al*, *J. Chem. Soc. C*, 1970, 1219 (*synth*)
Jose, C.I. *et al*, *Spectrochim. Acta*, 1973, **104**, 1394 (*ir*)
Khera, U. *et al*, *Indian J. Chem.*, *Sect. B*, 1978, **16**, 78 (*isol*)
Khera, U. *et al*, *Phytochemistry*, 1978, **17**, 596 (*Gentiobioside*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*rev, occur*)
Gupta, B.B. *et al*, *Phytochemistry*, 1983, **22**, 1306 (*isol*)

1,5,10-Trihydroxy-7-methoxy-3-methyl-1*H*-naphtho[2,3-*c*]pyran-6,9-dione T-80320

[119975-66-5]



$C_{15}H_{12}O_7$ M 304.256

Metab. of *Fusarium solani*. Deep purple cryst. (Me_2CO). Mp 245°.

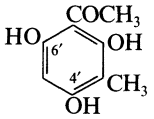
1-Me ether: [119975-67-6]. ***5,10-Dihydroxy-1,7-dimethoxy-3-methyl-1*H*-naphtho[2,3-c]pyran-6,9-dione***
$C_{16}H_{14}O_7$ M 318.282
Metab. of *F. solani*. Purple cryst. (C_6H_6). Mp 190°.

Tatum, J.H. *et al*, *Phytochemistry*, 1989, **28**, 283.

2′,4′,6′-Trihydroxy-3′-methylacetophenone T-80321

1-(2,4,6-Trihydroxy-3-methylphenyl)ethanone, 9CI

[2657-28-5]



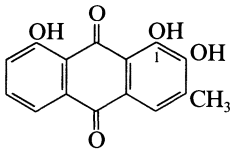
$C_9H_{10}O_4$ M 182.176

4′,6′-Di-Me ether: [23121-32-6]. *2′-Hydroxy-4′,6′-dimethoxy-3′-methylacetophenone.* ***Methylxanthoxylin***
$C_{11}H_{14}O_4$ M 210.229
Isol. from oil of *Acradenia franklinii* and from *Eugenia jambolana* (cloves). Light-yellow needles (pet. ether). Mp 143°.

Baldwin, M.E. *et al*, *Tetrahedron*, 1961, **16**, 206 (*isol, uv, synth*)
Cann, M.R. *et al*, *Chem. Ind.* (*London*), 1982, 779 (*pmr*)
Linde, H. *et al*, *Arch. Pharm.* (*Weinheim, Ger.*), 1983, **316**, 917 (*isol*)

1,2,8-Trihydroxy-3-methylanthraquinone T-80322

Norobtusifolin. 2-Hydroxychrysophanol



$C_{15}H_{10}O_5$ M 270.241

Constit. of *Myrsine africana* root. Orange-red needles (MeOH). Mp 265° (255°).

1-Me ether: [477-85-0]. ***Obtusifolin*†**
$C_{16}H_{12}O_5$ M 284.268
Isol. from seeds of *Cassia obtusifolia*. Yellow needles (MeOH). Mp 237-238°.

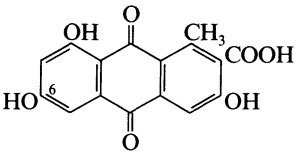
1-Me ether, di-Ac: Light-yellow needles. Mp 187-188°.

1-Me ether, O-β-D-Glucopyranosyl: ***Glucoobtusifolin***
$C_{22}H_{22}O_{10}$ M 446.410
Isol. from seeds of *Cassia obtusifolia*. Cryst + $1H_2O$. Mp 205-206°. Posn. of glucosylation not detd.

Tri-Me ether: 1,2,8-Trimethoxy-3-methylanthraquinone
$C_{18}H_{16}O_5$ M 312.321
Light-yellow needles (pet. ether). Mp 145-146°.

Takido, M., *Chem. Pharm. Bull.*, 1958, **6**, 397 (*isol, struct*)
Takido, M. *et al*, *CA*, 1963, **62**, 5326 (*Glucoobtusifolin*)
Li, X.-H. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 660 (*isol, pmr*)

3,6,8-Trihydroxy-1-methylanthraquinone-2-carboxylic acid T-80323



$C_{16}H_{10}O_7$ M 314.251

6-Me ether: [120374-28-9]. *3,8-Dihydroxy-6-methoxy-1-methylanthraquinone-2-carboxylic acid*
$C_{17}H_{12}O_7$ M 328.278
Constit. of *Gladiolus segetum*. Orange cryst. (MeOH). Mp 238-240°. Diagram incorrect in reference.

Ali, A.A. *et al*, *Phytochemistry*, 1989, **28**, 281.

3,4,6-Trihydroxy-2-methylbenzoic acid, 9CI T-80324

[27613-31-6]

$C_8H_8O_5$ M 184.148

Needles (MeOH aq.). Mp 192-193° dec.

Me ester:
$C_9H_{10}O_5$ M 198.175
Cryst. (MeOH). Mp 205°.

4,6-Di-Me ether: 3-Hydroxy-4,6-dimethoxy-2-methylbenzoic acid
$C_{10}H_{12}O_5$ M 212.202
Cryst. (C_6H_6). Mp 147-149° dec.

4,6-Di-Me ether, Me ester:
$C_{11}H_{14}O_5$ M 226.229
Long prisms (C_6H_6). Mp 114-115°.

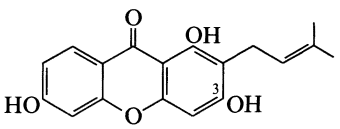
Tri-Me ether: [79786-37-1]. *3,4,6-Trimethoxy-2-methylbenzoic acid, 9CI*
$C_{11}H_{14}O_5$ M 226.229
Solid. Mp 149°.

Tri-Me ether, Me ester: 114992-40-4
$C_{12}H_{16}O_5$ M 240.255
Plates (Et_2O/hexane). Mp 70°.

Asahina, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1942, **17**, 152 (*synth*)
Evans, G.E. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 755 (*synth, uv, ir, pmr, ms*)

1,3,6-Trihydroxy-2-(3-methyl-2-butenyl)-9*H*-xanthen-9-one T-80325

1,3,6-Trihydroxy-2-prenylxanthone

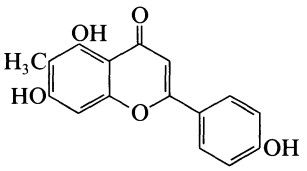


$C_{18}H_{16}O_5$ M 312.321

3-Me ether: [119227-98-4]. *1,6-Dihydroxy-3-methoxy-2-(3-methyl-2-butenyl)xanthone*
$C_{19}H_{18}O_5$ M 326.348
Constit. of *Garcinia mangostana*. Cryst. Mp >240°.

Parveen, M. *et al*, *Phytochemistry*, 1988, **27**, 3694.

4′,5,7-Trihydroxy-6-methylflavone T-80326

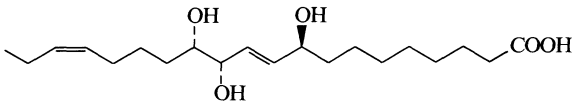


$C_{16}H_{12}O_5$ M 284.268

4′,7-Di-Me ether: 5-Hydroxy-4′,7-dimethoxy-6-methylflavone
$C_{18}H_{16}O_5$ M 312.321
Isol. from leaf wax of *Eucalyptus torrelliana* and *E. urnigera*. Cryst. ($CHCl_3$/pet. ether). Mp 187-188°.

Lamberton, J.A., *Aust. J. Chem.*, 1964, **17**, 692 (*isol, uv, ir, pmr, struct*)

9,12,13-Trihydroxy-10,15-octadecadienoic acid T-80327



$C_{20}H_{36}O_5$ M 356.501

(9S,10E,12S,13S,15Z)-form
Isol. from a resistant rice cultivar. Confers activity against rice blast disease.

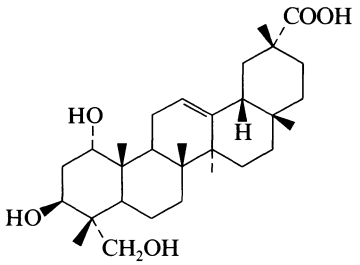
Me ester: $[\alpha]_D^{25}$ −10.90° (c, 1.01 in $CHCl_3$). Unnatural stereoisomers also synthesised.

*15,16-Dihydro: 9*S,12S,13S-*Trihydroxy*-10E-*octadecenoic acid*
$C_{20}H_{38}O_5$ M 358.517
Isol. from a rice cultivar. Confers resistance to rice blast disease.

15,16-Dihydro, Me ester: $[\alpha]_D^{25}$ −7.03° (c, 1.28 in $CHCl_3$). Unnatural stereoisomers also synthesised.

Suemune, H. *et al*, *Chem. Pharm. Bull.*, 1988, **36**, 3632 (*synth, ir, pmr, ms*)

1,3,23-Trihydroxy-12-oleanen-29-oic acid T-80328



$C_{30}H_{48}O_5$ M 488.706

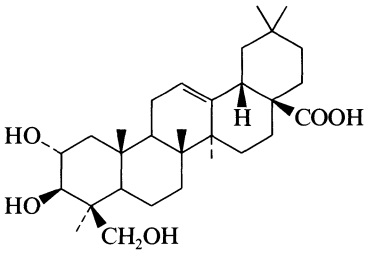
(1α,3β)-form
23-*Hydroxyimberbic acid*

*23-*O*-α-L-Rhamnopyranoside:* [118607-67-3].
$C_{36}H_{58}O_9$ M 634.849
Constit. of *Combretum imberbe*. Needles (EtOH). Mp 212-215°. $[\alpha]_D^{25}$ +12.9° (c, 1 in Py).

*1-Ac, 23-*O*-α-L-rhamnopyranoside:* [118607-68-4].
$C_{38}H_{60}O_{10}$ M 676.886
Constit. of *C. imberbe*. Prisms (EtOH). Mp 235-238°. $[\alpha]_D^{25}$ +5.6° (c, 0.6 in Py).

Rogers, C.B., *Phytochemistry*, 1988, **27**, 3217.

2,3,24-Trihydroxy-12-oleanen-28-oic acid T-80329



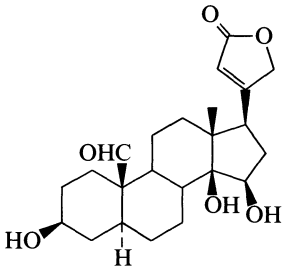
$C_{30}H_{48}O_5$ M 488.706

(2α,3β)-form [118711-55-0] ***Hyptatic acid* A**
Constit. of *Hyptis capitata*. Has anti-tumour activity. Cryst. Mp 298-304°. $[\alpha]_D^{20}$ +57° (c, 0.2 in MeOH).

Yamagishi, T. *et al*, *Phytochemistry*, 1988, **27**, 3213 (*isol, cryst struct*)

3,14,15-Trihydroxy-19-oxocard-20(22)-enolide T-80330

Updated Entry replacing A-00788

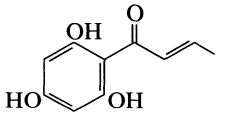


$C_{23}H_{32}O_6$ M 404.502

(3β,14β,5α,14β,15β)-form
Alloglaucotoxigenin
Aglycone from *Coronilla glauca*. Cryst. Mp 235° dec. $[\alpha]_D^{20}$ +27°.

Brandt, R. *et al*, *Helv. Chim. Acta*, 1966, **49**, 1662 (*uv, ir, pmr, ms, struct*)

1-(2,4,6-Trihydroxyphenyl)-2-buten-1-one T-80331



$C_{10}H_{10}O_4$ M 194.187

2,4-Di-Me ether: [119228-01-2]. *1-(2-Hydroxy-4,6-dimethoxyphenyl)-2-buten-1-one.* ***Verticilone***
$C_{12}H_{14}O_4$ M 222.240
Constit. of *Dysophyla verticillata*. Cryst. (hexane). Mp 79°.

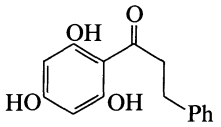
Tri-Me ether: [72896-76-5]. *1-(2,4,6-Trimethoxyphenyl)-2-buten-1-one.* ***Vertinone***
$C_{13}H_{16}O_4$ M 236.267
Constit. of *D. verticillata*. Cryst. (hexane/C_6H_6). Mp 95°.

Chakrabarti, A. *et al*, *Phytochemistry*, 1988, **27**, 3683.

1-(2,4,6-Trihydroxyphenyl)-3-phenyl-1-propanone T-80332

Updated Entry replacing U-30011

2′,4′,6′-Trihydroxydihydrochalcone



$C_{15}H_{14}O_4$ M 258.273

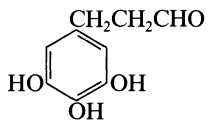
2-Me ether: [76444-56-9]. *1-(2,4-Dihydroxy-6-methoxyphenyl)-3-phenyl-1-propanone, 9CI. 2′,4′-Dihydroxy-6′-methoxydihydrochalcone.* ***Uvangoletin***
Isol. from *Uvaria angolensis*. Needles (EtOAc/pet. ether). Mp 189-190°.

4-Me ether: [35241-55-5]. *1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-1-propanone. 2′,6′-Dihydroxy-4′-methoxy-β-phenylpropiophenone*
$C_{16}H_{16}O_4$ M 272.300
Isol. from *Populus balsamifera* oil and from *Pitryogramma chrysophylla*. Light yellow needles (EtOH aq.). Mp 168°.

Tri-Me ether: 1-(2,4,6-Trimethoxyphenyl)-3-phenyl-1-propanone. 2′,4′,6′-Trimethoxydihydrochalcone
$C_{17}H_{18}O_4$ M 286.327
From *U. angolensis*. Cryst. ($CHCl_3$/hexane). Mp 74-76°.

Goris, A. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1935, **20**, 1435, 1520 (*isol, synth*)
Nilsson, M., *Acta Chem. Scand.*, 1961, **15**, 154 (*isol*)
Filho, R.B. *et al, Phytochemistry*, 1980, **19**, 1195 (*isol*)
Hufford, C.D. *et al, Phytochemistry*, 1980, **19**, 2036 (*isol*)
Bhardwaj, D.K. *et al, Indian J. Chem., Sect. B*, 1982, **21**, 476 (*synth*)

3-(3,4,5-Trihydroxyphenyl)propanal T-80333



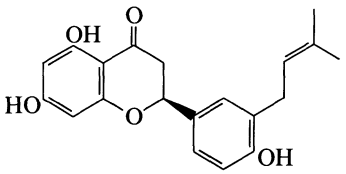
$C_9H_{10}O_4$ M 182.176

3,5-Di-Me ether: 3-(4-Hydroxy-3,5-dimethoxyphenyl)propanal. Dihydrosinapic aldehyde
$C_{11}H_{14}O_4$ M 210.229
Constit. of *Sorbus aucuparia*. Oil.

Malterud, K.E. *et al, Phytochemistry*, 1989, **28**, 1548.

4′,5,7-Trihydroxy-3′-prenylflavanone T-80334

2,3-Dihydro-5,7-dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4H-1-benzopyran-4-one, 9CI. 3′-Prenylnaringenin



$C_{20}H_{20}O_5$ M 340.375

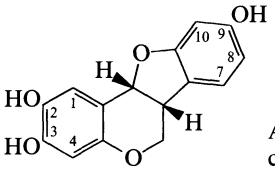
(S)-form [119240-82-3]
Constit. of *Erythrina eriotriocha*. Oil. $[\alpha]_D$ −1.1° (c, 2.2 in MeOH).

Nkengfack, A.E. *et al, J. Nat. Prod.* (*Lloydia*), 1989, **52**, 320 (*isol, pmr, cmr*)

2,3,9-Trihydroxypterocarpan T-80335

Updated Entry replacing H-01568

6a,11a-Dihydro-6H-benzofuro[3,2-c][1]benzopyran-2,3,9-triol



Absolute configuration

$C_{15}H_{12}O_5$ M 272.257

2,3-Di-Me ether: [73793-85-8]. *9-Hydroxy-2,3-dimethoxypterocarpan.* ***Sparticarpin***
$C_{17}H_{16}O_5$ M 300.310
Stress metab. from leaves of *Spartium japonicum*. $[\alpha]_D$ −170° approx. (c, 0.01 in MeOH).

2,9-Di-Me ether: [56752-00-2]. *3-Hydroxy-2,9-dimethoxypterocarpan. 2-Methoxymedicarpin*
$C_{17}H_{16}O_5$ M 300.310
Isol. from root crowns of *Pisum sativum*. Shows antifungal activity. Plates (Me_2CO). Mp 146-148°. $[\alpha]_D^{23}$ −297° (EtOH).

Tri-Me ether: [56782-49-1]. *2,3,9-Trimethoxypterocarpan. 2-Methoxyhomopterocarpin*
$C_{18}H_{18}O_5$ M 314.337
Isol. from *P. sativum*. Shows antibiotic props. Needles (C_6H_6/heptane). Mp 122-124°. $[\alpha]_D^{23}$ −228° (EtOH).

Kalra, V.K. *et al, Indian J. Chem.*, 1967, **5**, 607 (*synth*)
Pueppke, S.G. *et al, J. Chem. Soc., Perkin Trans.* 1, 1975, 946 (*isol*)
Ingham, J.L. *et al, Z. Naturforsch., C*, 1980, **35**, 197 (*Sparticarpin*)

3,4,9-Trihydroxypterocarpan T-80336

6a,11a-Dihydro-6H-benzofuro[3,2-c][1]benzopyran-3,4,9-triol. 4-Hydroxydemethylmedicarpin. 4′,7,8-Trihydroxypterocarpan

$C_{15}H_{12}O_5$ M 272.257
Isol. from fungus-infected leaves of *Melilotus alba*. Mp 118-120°.

9-Me ether: [53950-54-2]. *3,4-Dihydroxy-9-methoxypterocarpan. 4-Hydroxymedicarpin*
$C_{16}H_{14}O_5$ M 286.284
Isol. from fungus-infected leaves of *M. alba*.

3,9-Di-Me ether: 4-Hydroxy-3,9-dimethoxypterocarpan. 4-Hydroxyhomopterocarpin
$C_{17}H_{16}O_5$ M 300.310
Isol. from leaves of *Trifolium hydridum* and *T. pallescens* and from *M. alba* as fungal metab.

4,9-Di-Me ether: 3-Hydroxy-4,9-dimethoxypterocarpan. 4-Methoxymedicarpin
$C_{17}H_{16}O_5$ M 300.310
Constit. of *Swartzia madagascariensis, T. cherleri, T. pallescens* and *T. repens*. Prisms. Mp 158-160°. $[\alpha]_D$ −161° ($CHCl_3$).

Tri-Me ether: 3,4,9-Trimethoxypterocarpan. 4-Methoxyhomopterocarpin
$C_{18}H_{18}O_5$ M 314.337
Isol. from *Myroxylon peruiferum* and *Swartzia madagascariensis*. Needles (EtOH). Mp 118-120°.

(±)-form

4,9-Di-Me ether: [22973-33-7].
Cubes (C_6H_6/pet. ether). Mp 204-205°.

Tri-Me ether: Prisms (C_6H_6/pet. ether). Mp 114-115°.

Kalia, V.K. *et al, Tetrahedron*, 1967, **23**, 3221 (*synth*)

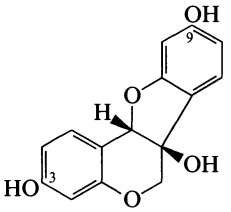
Campbell, R.V.M. *et al*, *J. Chem. Soc. C*, 1969, 1109 (*isol*)
Ingham, J.L., *Phytochemistry*, 1976, **15**, 1489 (*isol*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*occur*)

3,6*a*,9-Trihydroxypterocarpan T-80337

Updated Entry replacing T-30302

6H-Benzofuro[3,2-c][1]benzopyran-3,6a,9(11aH)-triol, 9CI. Glycinol

[69393-95-9]



Absolute configuration

$C_{15}H_{12}O_5$ M 272.257

Constit. of soybean seedlings (*Glycine max*). Also from *Erythrina sandwicensis* and *Pueraria thunbergiana*. λ_{max} 282 and 287 nm.

3-Me ether: 6a,9-*Dihydroxy*-3-*methoxypterocarpan*. 6a-*Hydroxyisomedicarpin*
$C_{16}H_{14}O_5$ M 286.284
Isol. from fungus-infected leaves of *Melilotus alba*.

9-Me ether: [61135-92-0]. *3,6a-Dihydroxy-9-methoxypterocarpan*. 6a-*Hydroxymedicarpin*
$C_{16}H_{14}O_5$ M 286.284
Isol. from fungus-infected leaves of *M. alba* and *Trifolium pratense*.

3,9-Di-Me ether: [3187-52-8]. 6a-*Hydroxy*-3,9-*dimethoxypterocarpan*. ***Variabilin*†**. *Homopisatin*
$C_{17}H_{16}O_5$ M 300.310
Isol. from wood of *Dalbergia variabilis*. Stress metab. from leaves or colyledons of *Caragana* spp., *Lathyrus* spp., *Lens culinaris*, *L. nigricans*, *Parochetus communis* and *T. pratense*.

Ingham, J.L., *Phytochemistry*, 1976, **15**, 1489 (*isol*)
Kurosawa, K. *et al*, *Phytochemistry*, 1978, **17**, 1417 (*Variabilin*)
Ingham, J.L., *Z. Naturforsch.*, *C*, 1980, **35**, 384 (*isol*)
Weistein, L.I. *et al*, *Plant Physiol.*, 1981, **68**, 358 (*isol*)
Ingham, J.L., *Fortschr. Chem. Org. Naturst.*, 1983, **43**, 1 (*occur*)

3,9,10-Trihydroxypterocarpan T-80338

6a,11a-Dihydro-6H-benzofuro[3,2-c][1]benzopyran-3,9,10-triol, 9CI

$C_{15}H_{12}O_5$ M 272.257

9-Me ether: [69853-46-9]. *3,10-Dihydroxy-9-methoxypterocarpan*. ***Vesticarpan***
$C_{16}H_{14}O_5$ M 286.284
Isol. from *Machaerium vestitum* and *Platymiscium trinitatis* woods. Cryst. (MeOH). Mp 154-156°. Opt. active (6*a*S,11*a*S). Also descr. as an oil.

10-Me ether: [73340-42-8]. *3,9-Dihydroxy-10-methoxypterocarpan*. ***Nissolin***
$C_{16}H_{14}O_5$ M 286.284
Isol. from phyllodes of *Lathyrus nissolia*.

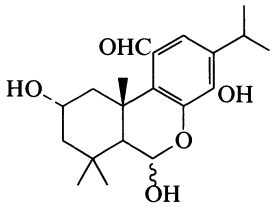
9,10-Di-Me ether: [73340-41-7]. *3-Hydroxy-9,10-dimethoxypterocarpan*. ***Methylnissolin***
$C_{17}H_{16}O_5$ M 300.310
Isol. from phyllodes of *L. nissolia* (stress metab.).

(±)-form

9-Me ether: Microcryst. Mp 121°.

Craveiro, A.A. *et al*, *Phytochemistry*, 1974, **13**, 1629 (*Vesticarpan*)
Kurosawa, K. *et al*, *Phytochemistry*, 1978, **17**, 1413 (*Vesticarpan*)
Robeson, J.D. *et al*, *Phytochemistry*, 1979, **18**, 1715 (*Nissolin*, *Methylnissolin*)

2,11,12-Trihydroxy-6,7-seco-8,11,13-abietatriene-6,7-dial 11,6-hemiacetal T-80339



$C_{20}H_{28}O_5$ M 348.438

Not named in the paper.

2α-form

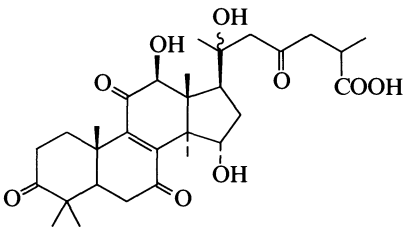
Constit. of *Salvia texana*. Oil. Mixt. of 6-epimers.

Tri-Ac(6α-): [122558-74-1].
$C_{26}H_{34}O_8$ M 474.550
Constit. of *S. texana*.

[122558-70-7, 122558-71-8]

Gonzalez, A.G. *et al*, *J. Chem. Res.* (*S*), 1989, 132.

12,15,20-Trihydroxy-3,7,11,23-tetraoxo-8-lanosten-26-oic acid T-80340



$C_{30}H_{42}O_9$ M 546.656

(12β,15α,20ξ)-form [120462-50-2] ***Ganoderic acid AP***

Constit. of *Ganoderma applantum*.

Me ester: $[\alpha]_D^{23}$ +71° (c, 0.2 in EtOH).

Nishitoba, T. *et al*, *Phytochemistry*, 1989, **28**, 193.

4′,5,7-Trihydroxy-3′,6,8-trimethoxyflavone T-80341

5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6,8-dimethoxy-4H-1-benzopyran-4-one, 9CI. ***Sudachitin***. *Majoranin*

[4281-28-1]

$C_{18}H_{16}O_8$ M 360.320

Constit. of *Citrus sudachi* and *Majorana hortensis*. Yellow needles (MeOH). Mp 241-243°.

4′-O-β-D-Glucopyranoside: [70575-17-6]. ***Sudachiin A***
$C_{24}H_{26}O_{13}$ M 522.462
Constit. of *C. sudachi*. Yellow needles (MeOH). Mp 211-213°. $[\alpha]_D$ −37.4° (c, 0.31 in 0.5% NaOH aq.).

7-O-β-D-Glucopyranoside: [70575-23-4].
$C_{24}H_{26}O_{13}$ M 522.462
Constit. of *Sideritis leucantha*. Yellow needles (MeOH). Mp 187-188°. $[\alpha]_D$ +58.9° (c, 0.26 in 0.51% NaOH aq.).

Horie, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1961, **34**, 1547 (*isol*)
Horie, T. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1962, **83**, 468 (*synth*)
Lee, H.H. *et al*, *J. Chem. Soc.*, 1964, 6255 (*synth*)
Mabry, T.J. *et al*, *Curr. Sci.*, 1972, **41**, 202 (*isol*, *struct*)
Tomas, F. *et al*, *Phytochemistry*, 1980, **19**, 2039.
Horie, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 2928 (*isol*, *synth*)

2,3,19-Trihydroxy-12-ursen-28-oic acid T-80342

Updated Entry replacing T-03537

$C_{30}H_{48}O_5$ M 488.706

(2α,3α,19α)-form [53155-25-2]

Constit. of *Pygeum acuminatum*. Cryst. (MeOH). Mp 264°.

(2α,3β,19α)-form [13850-16-3] ***Tormentic acid***

Aglycone from Tormentoside from *Potentilla tormentilla*. Cryst. Mp 273°. $[\alpha]_D$ −20° (Py).

28-O-β-D-Glycopyranoside: [88515-58-6]. *Tormentic acid ester glucoside*

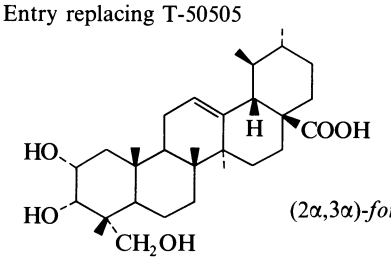
$C_{36}H_{58}O_{10}$ M 650.848

Constit. of *Rosa multiflora* and *Aphloia theiformis*. Amorph. powder.

Potier, P. *et al*, *Bull. Soc. Chim. Fr.*, 1966, **11**, 3458 (*isol*)
Chandel, R.S. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 914 (*isol*)
Gopalsamy, N. *et al*, *Phytochemistry*, 1988, **27**, 3593 (*deriv*)

2,3,23-Trihydroxy-12-ursen-28-oic acid T-80343

Updated Entry replacing T-50505



(2α,3α)-*form*

$C_{30}H_{48}O_5$ M 488.706

(2α,3α)-form [76964-07-3] ***Esculentic acid***†

Constit. of *Nepeta hindostana*, *Diplazium esculentum*, *Hedyotis lawsoniae* and *Prunella vulgaris*. Cryst. (MeOH). Mp 270°.

(2α,3β)-form [464-92-6] ***Asiatic acid***

Constit. of *Dipterocarpus pilosus* and *Dryobalanops aromatica*. Cryst. by subl. Mp 300-305°.

▷ Causes exp. neoplasms.

Me ester: Cryst. (C_6H_6). Mp 224-225.5°. $[\alpha]_D$ +54.5°.

28-[6-Deoxy-α-L-mannopyranosyl-(1→4)-O-β-D-glucopyranosyl-(1→6)-O-β-D-glucopyranoside]: [16830-15-2]. ***Asiaticoside.*** *Blastostimulina. Centelase. Emdecassol. Madecassol. Marticassol. FK 1080*

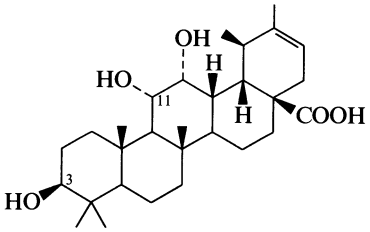
$C_{48}H_{78}O_{19}$ M 959.133

Constit. of *Centella asiatica*. Shows antibiotic activity against gram-positive organisms and mycobacteria, particularly *M.tuberculosis*. Used in wound therapy. Cryst. Mp 235-238° (230-233°). $[\alpha]_D^{20}$ −14° (EtOH).

▷ YU9625000.

Polonsky, J. *et al*, *Bull. Soc. Chim. Fr.*, 1959, 880 (*isol*)
Polonsky, J. *et al*, *Bull. Soc. Chim. Fr.*, 1961, 1586 (*struct*)
Singh, B. *et al*, *Phytochemistry*, 1969, **8**, 917 (*isol*)
Chasseaud, L.F. *et al*, *Arzneim.-Forsch.*, 1971, **21**, 1379 (*metab*, *Asiaticoside*)
Gupta, A.S. *et al*, *Tetrahedron*, 1971, **27**, 823 (*isol*)
Velasco, M. *et al*, *Curr. Ther. Res., Clin. Exp.*, 1976, **19**, 121 (*Asiaticoside*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 1600.
Ahmad, V.U. *et al*, *Phytochemistry*, 1986, **25**, 1487 (*isol*)
Kojima, H. *et al*, *Phytochemistry*, 1989, **28**, 1703 (*pmr*, *struct*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 6th Ed., Van Nostrand-Reinhold, 1984, 326.

3,11,12-Trihydroxy-20-ursen-28-oic acid T-80344



$C_{30}H_{48}O_5$ M 488.706

(3β,11α,12α)-form

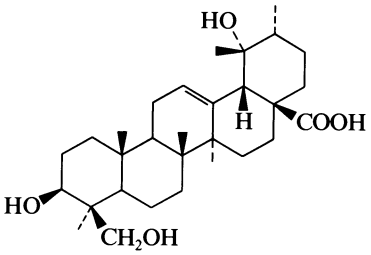
3-O-(4-Hydroxyphenyl), 11-Me-ether: ***Oleanderolic acid***

$C_{37}H_{54}O_5$ M 578.831

Constit. of *Nerium oleander*. Cryst. (EtOAc/pet. ether). Mp 262-264°. $[\alpha]_D^{24}$ +50.0° (c, 0.04 in $CHCl_3$).

Siddiqui, S. *et al*, *Phytochemistry*, 1989, **28**, 1187.

3,19,24-Trihydroxy-12-ursen-28-oic acid T-80345



$C_{30}H_{48}O_5$ M 488.706

(3β,19α)-form

Rotungenic acid

Constit. of *Ilex rotunda*. Cryst. (MeOH aq.). Mp 295-298° dec. $[\alpha]_D$ +16° (MeOH).

Nakatani, M. *et al*, *Phytochemistry*, 1989, **28**, 1479.

3,6,19-Trihydroxy-12-ursen-28-oic acid T-80346

$C_{30}H_{48}O_5$ M 488.706

(3β,6β,19α)-form

Constit. of *Uncaria florida*. Cryst. (MeOH aq.). Mp 226-227°.

Me ester: Cryst. (MeOH aq.). Mp 220-221°.

Aimi, N. *et al*, *Tetrahedron*, 1989, **45**, 4125.

1,3,7-Trihydroxyxanthone T-80347

Updated Entry replacing T-20280

1,3,7-Trihydroxy-9H-xanthen-9-one, 9CI. ***Gentisein***

[529-49-7]

$C_{13}H_8O_5$ M 244.203

Isol. from *Gentiana lutea*. Orange-yellow needles (MeOH). Mp 321-323°.

Tri-Ac:

$C_{19}H_{14}O_8$ M 370.315

Mp 229-230°.

1-Me ether: [16850-68-3]. *3,7-Dihydroxy-1-methoxyxanthone*

$C_{14}H_{10}O_5$ M 258.230

Yellow needles (MeOH aq.). Mp 178°.

3-Me ether: [437-50-3]. *1,7-Dihydroxy-3-methoxyxanthone.* ***Gentisin.*** *Gentianin. Gentianic acid*

$C_{14}H_{10}O_5$ M 258.230

Pigment from root of *G. lutea*. Yellow needles. Mp 273-275° (266-267°).

▷ ZD6034600.

3-Me ether, 7-glucoside:
$C_{20}H_{20}O_{10}$ M 420.372
From *G. verna*. Mp 219-222° dec.

3-Me ether, 1-O-primeveroside: 7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone
$C_{25}H_{28}O_{14}$ M 552.488
Constit. of *G. lutea*. Needles. Mp 259-260° dec. $[\alpha]_D^{20}$ −81.5° (c, 0.4 in Py).

3-Me ether, 7-O-primeveroside: 1-Hydroxy-3-methoxy-7-primeverosyloxyxanthone
$C_{25}H_{28}O_{14}$ M 552.488
Constit. of *G. lutea*. Needles. Mp 293-294° dec. $[\alpha]_D^{20}$ −69.4° (c, 0.36 in Py).

7-Me ether: [491-64-5]. *1,3-Dihydroxy-7-methoxyxanthone.* ***Isogentisin***
$C_{14}H_{10}O_5$ M 258.230
Mp 241°.
▷ ZD6034500.

7-Me ether, 3-O-primeveroside: [529-48-6]. ***Gentioside.*** *1-Hydroxy-7-methoxy-3-primeverosyloxyxanthone*
$C_{25}H_{28}O_{14}$ M 552.488
Constit. of *G. lutea*. Needles. Mp 278-279° dec. $[\alpha]_D^{20}$ −50° (c, 0.3 in Py).

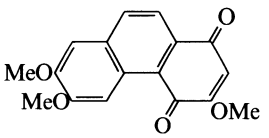
3,7-Di-Me ether: [13379-35-6]. *1-Hydroxy-3,7-dimethoxyxanthone*
$C_{15}H_{12}O_5$ M 272.257
Isol. from *G. lutea* and *Frasera albicaulis*. Cryst. (MeOH), yellow needles (CH_2Cl_2/hexane). Mp 169-170°.

Tri-Me ether: [3722-54-1]. *1,3,7-Trimethoxyxanthone*
$C_{16}H_{14}O_5$ M 286.284
Cryst. (EtOAc). Mp 173-174°.

Shinoda, J., *J. Chem. Soc.*, 1927, 1985 (*synth*)
Atkinson, J.E. *et al*, *Tetrahedron*, 1969, **25**, 1507 (*isol, synth*)
Stout, G.H. *et al*, *Tetrahedron*, 1969, **25**, 1961 (*isol, synth*)
Chawla, H.M. *et al*, *Proc.-Indian Acad. Sci., Sect. A*, 1973, **78**, 141 (*ir*)
Hostettmann, K. *et al*, *Helv. Chim. Acta*, 1974, **57**, 1155 (*isol*)
Ellis, R.C. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1976, 1377 (*synth*)
Chadha, R. *et al*, *Indian J. Chem., Sect. A*, 1979, **18**, 505 (*cmr*)
Fram, A.W. *et al*, *Tetrahedron*, 1979, **35**, 2035 (*cmr*)
Hayashi, T. *et al*, *Phytochemistry*, 1988, **27**, 3696 (*derivs*)

3,6,7-Trimethoxy-1,4-phenanthraquinone T-80348

Sphenone A



$C_{17}H_{14}O_5$ M 298.295
Constit. of *Sphenomeris biflora*. Cytotoxic substance. Orange granules ($CHCl_3$). Mp 235-238°.

Wu, T.-S. *et al*, *Phytochemistry*, 1989, **28**, 1280.

2,3,5-Trimethylbenzyl alcohol T-80349

2,3,5-Trimethylbenzenemethanol, 9CI
[50849-01-9]
$C_{10}H_{14}O$ M 150.220
Cryst. (hexane). Mp 50-51°.

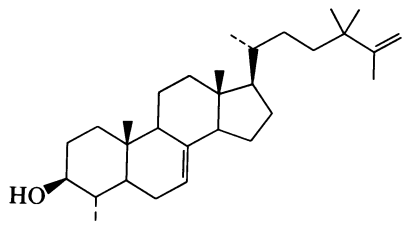
Baciocchi, E. *et al*, *J. Org. Chem.*, 1977, **42**, 3682; 1980, **45**, 3906 (*synth, deriv, pmr*)

3,4,5-Trimethylbenzyl alcohol T-80350

3,4,5-Trimethylbenzenemethanol, 9CI
[39126-11-9]
$C_{10}H_{14}O$ M 150.220
Needles (pet.ether). Mp 72-74°.

Suzuki, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1969, **42**, 2618 (*synth*)
Baciocchi, E. *et al*, *J. Org. Chem.*, 1977, **42**, 3682 (*deriv, pmr*)
Kim, E.K. *et al*, *J. Org. Chem.*, 1989, **54**, 1692 (*ir, pmr*)

4,24,24-Trimethyl-7,25-cholestadien-3-ol T-80351

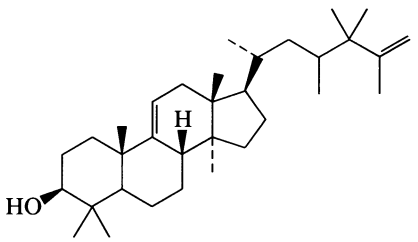


$C_{30}H_{50}O$ M 426.724

(3β,4α,5α)-form
Erianol
Constit. of *Eria convallarioides*. Cryst. (EtOAc/pet. ether). Mp 168°. $[\alpha]_D$ +3.5° ($CHCl_3$).

Majumder, P.L. *et al*, *Phytochemistry*, 1989, **28**, 1487.

23,24,24-Trimethyl-9(11),25-lanostadien-3-ol T-80352



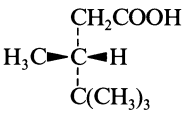
$C_{33}H_{56}O$ M 468.805

3β-form [62462-35-5] ***Lansiol***
Constit. of *Clausena lansium*. Cryst. ($CHCl_3$/MeOH). Mp 197-198°. $[\alpha]_D^{25}$ +83° (c, 1 in $CHCl_3$).

Lakshmi, V. *et al*, *Phytochemistry*, 1989, **28**, 943.

3,4,4-Trimethylpentanoic acid, 9CI T-80353

[75177-71-8]



(R)-form

$C_8H_{16}O_2$ M 144.213

(R)-form [40824-44-0]
Oil. $[\alpha]_D^{25}$ +21.7° (c, 0.9 in EtOH).

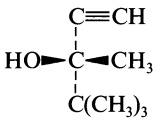
Chloride:
$C_8H_{15}ClO$ M 162.659
Bp_{30} 85°.

(±)-form
Bp_{18} 126°, Bp_4 90°.
[64043-89-6]

Menicagli, R. *et al*, *J. Chem. Res.* (*S*), 1978, 262 (*synth*)
Azzena, U. *et al*, *Helv. Chim. Acta*, 1981, **64**, 2821 (*synth, resoln, pmr, cmr*)
Zhang, W.-Y. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4652 (*synth, ir, pmr, cmr*)

3,4,4-Trimethyl-1-pentyn-3-ol, 9CI T-80354

[993-53-3]



(*S*)-*form*

$C_8H_{14}O$ M 126.198

Abs. config. controversial. Now almost certainly established.

(*S*)-*form* [38484-41-2]

Liq. Bp_{15} 45-47°. $[\alpha]_D^{20}$ +0.06° (neat), $[\alpha]_D^{20}$ +0.78° (c, 1.1 in CH_2Cl_2).

(±)-*form*

Liq. d_4^{20} 1.06. Bp_{11} 76-76.5°.

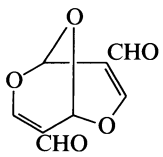
Hydrazide: Cryst. (EtOAc/EtOH). Mp 91-92°.

[38484-42-3, 104758-84-1]

Caporusso, A.M. *et al*, *Gazz. Chim. Ital.*, 1986, **116**, 467 (*cd*)
Elsevier, C.J. *et al*, *J. Org. Chem.*, 1987, **52**, 1536 (*synth, ir, nmr*)
Eliel, E.L. *et al*, *Tetrahedron Lett.*, 1987, **28**, 4813 (*abs config*)

2,6,9-Trioxabicyclo[3.3.1]nona-3,7-diene-4,8-dicarboxaldehyde, 9CI T-80355

[116149-12-3]



$C_8H_6O_5$ M 182.132

(±)-*form*

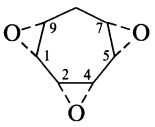
Prod. of treatment of triformylmethane with $COCl_2$. Cryst. (1,2-dichloroethane). Mp 180°. Sublimes. Previous proposed struct. incorrect.

Arnold, Z. *et al*, *J. Org. Chem.*, 1988, **53**, 5352 (*synth, ms, ir, pmr, cmr*)

3,6,10-Trioxatetracyclo[7.1.0.0^{2,4}.0^{5,7}]decane, 9CI T-80356

Updated Entry replacing T-04249

Trioxatris-σ-homotropilidene



(1α,2α,4α,5α,7α,9α)-*form*

$C_7H_8O_3$ M 140.138

(*1α,2α,4α,5α,7α,9α*)-*form* [59992-00-6]

syn,syn-*form*

Cryst. Mp 165°.

(*1α,2α,4α,5β,7β,9α*)-*form* [61687-82-9]

syn,anti-*form*

Plates (CH_2Cl_2/Et_2O). Mp 66-67°.

(*1α,2β,4β,5α,7α,9α*)-*form* [61664-66-2]

anti,anti-*form*

Needles (CH_2Cl_2/pentane). Mp 110-112°.

(*1α,2β,4β,5α,7α,9α*)-*form*

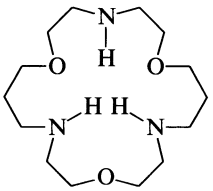
anti,anti-*form*

Needles (CH_2Cl_2/pentane). Mp 110-112°.

Prinzbach, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1976, **15**, 559 (*synth, pmr, cmr*)
Adam, W. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 1961 (*synth, ir, pmr, cmr*)
Sütbeyaz, Y. *et al*, *J. Org. Chem.*, 1988, **53**, 2312 (*synth*)

1,7,14-Trioxa-4,11,17-triazacycloeicosane, 9CI T-80357

[116073-75-7]



$C_{14}H_{31}N_3O_3$ M 289.417

Oil.

4,11,17-Tri-Me: [116073-76-8].

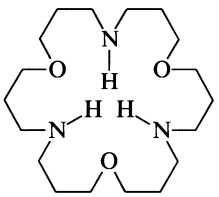
$C_{17}H_{37}N_3O_3$ M 331.498

Oil.

Pratt, J.A.E. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 13 (*synth, pmr*)

1,9,17-Trioxa-5,13,21-triazacyclotetracosane, 9CI T-80358

[116073-69-9]



$C_{18}H_{39}N_3O_3$ M 345.524

B,3HCl: [116073-96-2].

Cryst. (EtOH/Et_2O). Mp 250°. Hygroscopic.

5,13,21-Tri-Me: [116073-70-2].

$C_{21}H_{45}N_3O_3$ M 387.605

Oil.

Pratt, J.A.E. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1988, 13 (*synth, pmr*)

Triphenylacetaldehyde T-80359

α,α-Diphenylbenzeneacetaldehyde, 9CI. 2,2,2-Triphenylethanal

[42365-04-8]

Ph_3CCHO

$C_{20}H_{16}O$ M 272.346

Cryst. Mp 105.5°.

Oxime: [41401-04-1].

$C_{20}H_{17}NO$ M 287.360

Cryst. Mp 190°.

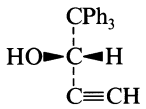
Semicarbazone: Cryst. Mp 223°.

Phenylhydrazone: Cryst. Mp 142°.

Daniloff, S., *Russ. J. Phys. Chem.*, 1917, **49**, 282; *CA*, **18**, 1488 (*synth, deriv*)
Daniloff, S. *et al*, *Ber.*, 1926, **59**, 377 (*synth, deriv*)
Henderson, M.A. *et al*, *J. Org. Chem.*, 1988, **53**, 4736 (*synth, ir, pmr, cmr*)

1,1,1-Triphenyl-3-butyn-2-ol T-80360

α-Ethynyl-β,β-diphenylbenzeneethanol, 9CI. Ethynyltritylcarbinol



(S)-form

$C_{22}H_{18}O$ M 298.384

(S)-form [115648-30-1]
Cryst. (Et_2O). Mp 92-93°. $[\alpha]_D^{22}$ −9.81° (c, 0.031 in $CHCl_3$).

(±)-form [115533-97-6]
Cryst. Mp 80-82°.

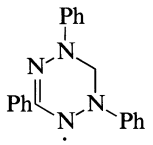
[115648-31-2]

Henderson, M.A. *et al*, *J. Org. Chem.*, 1988, **53**, 4736 (*synth, resoln, ir, pmr, cmr*)

2,4,6-Triphenyl-3,4-dihydro-1,2,4,5-tetrazin-1(2*H*)-yl, 9CI T-80361

2,4,6-Triphenylverdazyl. 1,3,5-Triphenylverdazyl

[2154-65-6]



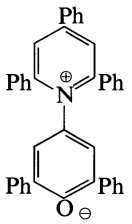
$C_{20}H_{17}N_4$ M 313.381
Radical scavenger. Blue-black cryst. (MeOH). Green in soln. or melt. Mp 161°.

Kuhn, R. *et al*, *Monatsh. Chem.*, 1964, **95**, 457 (*synth, uv, ir, esr*)
Williams, D.E., *Acta Crystallogr., Sect. B*, 1973, **29**, 96 (*cryst struct*)

2,4,6-Triphenyl-*N*-(3,5-diphenyl-4-oxidophenyl)pyridinium betaine T-80362

1-(2′-Hydroxy[1,1′:3′,1″-terphenyl]-5′-yl)-2,4,6-triphenylpyridinium hydroxide inner salt,9CI. 2,4,6-Triphenylpyridinium 4-oxo-3,5-diphenyl-2,5-cyclohexadien-1-ylide. Reichardt's dye

[10081-39-7]



$C_{41}H_{29}NO$ M 551.686
Used in determination of solvent polarity (Kosower Z values). Violet-black cryst. + $2H_2O$ (MeOH aq.). Mp 205-276° dec. Highly solvatochromic.

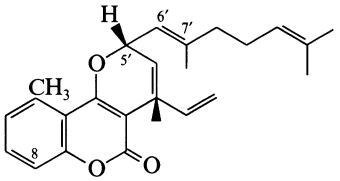
B, $HClO_4$: Yellow plates (AcOH or MeOH). Mp 273-274°.

[43085-74-1]

Dimroth, K. *et al*, *Justus Liebigs Ann. Chem.*, 1963, **661**, 1 (*synth, ir, uv, derivs*)
Reichardt, C. *et al*, *Justus Liebigs Ann. Chem.*, 1983, 721 (*props, use, bibl*)
Johnson, B.P. *et al*, *Anal. Lett.*, 1986, **19**, 939 (*synth, props, use*)
Kessler, M.A. *et al*, *Synthesis*, 1988, 635 (*synth*)

Triptiliocoumarin T-80363

[119365-36-5]



$C_{25}H_{30}O_3$ M 378.510
Constit. of *Triptilion benaventei*. Gum. $[\alpha]_D^{24}$ −22° (c, 0.16 in $CHCl_3$).

5′-Hydroxy: [119478-83-0]. ***5′-Hydroxytriptiliocoumarin***
$C_{25}H_{30}O_4$ M 394.510
Constit. of *T. benaventei*. Gum.

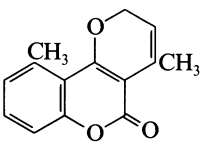
8-Hydroxy: [118555-92-3]. ***8-Hydroxytriptiliocoumarin***
$C_{25}H_{30}O_4$ M 394.510
Constit. of *T. benaventei*. Gum. $[\alpha]_D^{24}$ +8° (c, 0.18 in $CHCl_3$).

5′-Epimer, 5′-hydroxy, 6′,7′-epoxide: [118555-93-4]. ***6′,7′-Epoxy-5′α-hydroxytriptiliocoumarin***
$C_{25}H_{30}O_5$ M 410.509
Constit. of *T. benaventei*. Gum.

Bittner, M. *et al*, *Phytochemistry*, 1988, **27**, 3263.

Triptispinocoumarin T-80364

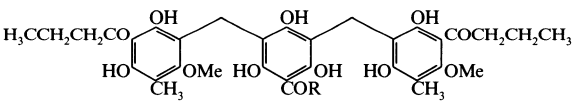
[118227-65-9]



$C_{14}H_{12}O_3$ M 228.247
Constit. of *Triptilion spinosum*. Gum.

Bittner, M. *et al*, *Phytochemistry*, 1988, **27**, 3263.

Trisaemulins T-80365



Trisaemulin BAB (R = CH_3)

Trisaemulin BBB (R = $CH_2CH_2CH_3$)

The suffixes refer to the acyl sidechains (A = acetyl, B = butyryl). Isol. from *Dryopteris aemula* and poss. present in *D. crispifolia*.

Trisaemulin BAB [56226-94-9]
$C_{34}H_{40}O_{12}$ M 640.683
Mp 180-183°. Not completely pure of BBB.

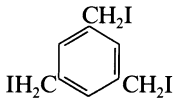
Trisaemulin BBB [49582-13-0]
$C_{36}H_{44}O_{12}$ M 668.736
Mp 168-170°. Not completely pure of BAB.

Widén, C.-J. *et al*, *Helv. Chim. Acta*, 1975, **58**, 881 (*isol, ms, pmr, struct*)

1,3,5-Tris(iodomethyl)benzene, 9CI T-80366

ω,ω′,ω″-Triiodomesitylene

[90678-60-7]



$C_9H_9I_3$ M 497.884

Cryst. (pet. ether/toluene). Mp 133-134°.

Reiche, W.S. *et al*, *J. Chem. Soc.*, 1947, 1234 (*synth*)
Bilger, C. *et al*, *Synthesis*, 1988, 902 (*synth*)

Tris(methylthio)methylium(1+), 9CI T-80367

$(MeS)_3C^{\oplus}$

$C_4H_9S_3^{\oplus}$ M 153.313 (ion)

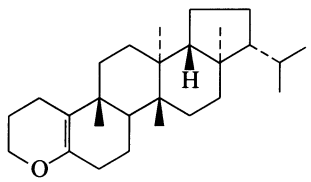
Methylsulfate: [116538-66-0].
$C_5H_{12}O_4S_4$ M 264.411
Solid. Mp 66-67°. Extremely moisture sensitive.

Tetrafluoroborate: [18702-35-7].
$C_4H_9BF_4S_3$ M 240.118
Cryst. (Et_2O/MeCN). Mp 168-170°. Can be stored at low temp. and dry conditions.

Tucker, W.P. *et al*, *Tetrahedron Lett.*, 1967, 2747 (*synth, pmr*)
Barbero, M. *et al*, *Synthesis*, 1988, 22 (*synth, pmr, cmr, use, bibl*)

Trisnorisoespinenoxide T-80368

3,4-Seco-4,23,24-trisnor-D:B-friedo-B′:A′-neogammacer-5(10)-ene 3,5-oxide



$C_{27}H_{44}O$ M 384.644

Constit. of *Euphorbia supina*. Cryst. Mp 209-213°. $[\alpha]_D^{23}$ −2.9° (c, 0.63 in $CHCl_3$).

Tanaka, R. *et al*, *Tetrahedron Lett.*, 1989, **30**, 1661.

Tritriacontane T-80369

[630-05-7]

$H_3C(CH_2)_{31}CH_3$

$C_{33}H_{68}$ M 464.900

Isol. from many plant waxes incl. Candelilla wax. Major constit. of some waxes, e.g. *Agave sisalana* (33%), *Calocephalus brownii* (12%). Mp 71.8°. Four crystal modifications known.

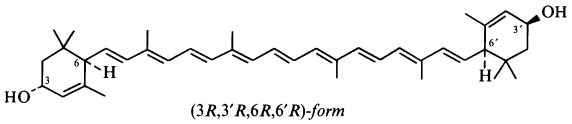
Chibnall, A.C. *et al*, *Biochem. J.*, 1934, **28**, 2189.
Razafindrazaka, J. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1633 (*isol*)
Batterham, T.J. *et al*, *Aust. J. Chem.*, 1966, **19**, 143 (*isol*)
Piesczek, W. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 1278 (*cryst struct*)

Tunaxanthin T-80370

Updated Entry replacing C-00615

ε,ε-Carotene-3,3′-diol, 9CI

[12738-95-3]



(3*R*,3′*R*,6*R*,6′*R*)-*form*

$C_{40}H_{56}O_2$ M 568.881

Various stereoisomers occur as fish and crustacean pigments.

3-Epimer: Chiriquixanthin B
From *A. chiriquiensis*.

(3R,3′R,6R,6′R)-form [78306-12-4]
Tunaxanthin F. Lactucaxanthin

(3R,3′R,6R,6′S)-form [97673-78-4]
Tunaxanthin H

(3R,3′R,6S,6′S)-form [71697-13-7]
Tunaxanthin C. Oxyxanthin 58

(3R,3′S,6R,6′R)-form [63597-82-0]
Tunaxanthin I. Chiriquixanthin A
Also isol. from the skin of *Atelopus chiriquiensis*.

(3R,3′S,6R,6′S)-form [82915-90-0]
Tunaxanthin E

(3R,3′S,6S,6′R)-form [82915-89-7]
Tunaxanthin D

(3R,3′S,6S,6′S)-form [72274-50-1]
Tunaxanthin B. Oxyxanthin 51

(3S,3′S,6R,6′R)-form [63597-83-1]
Tunaxanthin J. Chiriquixanthin B
Also isol. from skin of *A. chiriquiensis*.

(3S,3′S,6R,6′S)-form [97746-99-1]
Tunaxanthin G

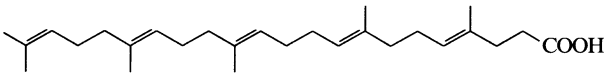
(3S,3′S,6S,6′S)-form [71697-14-8]
Tunaxanthin A

[82915-92-2, 83148-14-5]

Bingham, A. *et al*, *J. Chem. Soc. C*, 1977, 96 (*Chiriquixanthins*)
Rønneberg, H. *et al*, *Acta Chem. Scand., Ser. B*, 1978, **32**, 621 (*struct, pmr, ms, uv, cd, abs config*)
Matsuno, T. *et al*, *CA*, 1983, **100**, 85953u; 1984, **101**, 207845d (*isol*)
Ikano, Y. *et al*, *J. Chromatogr.*, 1985, **328**, 387 (*hplc*)

Turbinaric acid T-80371

4,8,13,17,21-Pentamethyl-4,8,12,16,20-docosapentaenoic acid



$C_{27}H_{46}O_2$ M 402.659

Constit. of *Turbinaria ornata*.

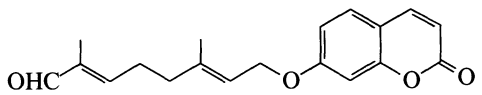
van Tamelen, E.E. *et al*, *Tetrahedron Lett.*, 1962, 121 (*synth*)
Asari, F. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1167 (*isol, pmr, cmr*)

U

Umbelliferone 8-oxogeranyl ether U-80001

2,6-Dimethyl-8-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-2,6-octadienal, 9CI

[30825-46-8]



$C_{19}H_{20}O_4$ M 312.365

Isol. from *Capnophyllium peregrinum*. Cryst. (Et_2O/pet. ether). Mp 64°.

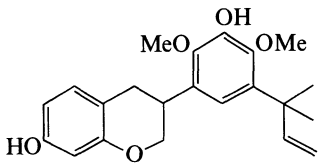
Bohlmann, F. *et al*, *Chem. Ber.*, 1970, **103**, 3619; 1974, **107**, 1780.

Unanisoflavan U-80002

Updated Entry replacing U-00024

3-[5-(1,1-Dimethyl-2-propenyl)-3-hydroxy-2,4-dimethoxyphenyl]-3,4-dihydro-2H-1-benzopyran-7-ol, 9CI. 5'-(1,1-Dimethylallyl)-3',7-dihydroxy-2',4'-dimethoxyisoflavan

[61186-60-5]



$C_{22}H_{26}O_5$ M 370.444

(−)-form

Constit. of *Sophora secondiflora*. Mp 184°. $[\alpha]_D$ −73.5° ($CHCl_3$).

4'-O-De-Me: [58210-35-8]. ***α,α-Dimethylallylcyclolobin.*** *4-(3,4-Dihydro-7-hydroxy-2H-1-benzopyran-3-yl)-6-(1,1-dimethyl-2-propenyl)-3-methoxy-1,2-benzenediol, 9CI*

$C_{21}H_{24}O_5$ M 356.418

Isol. from *Cyclobium clausseni* heartwood. Needles. Mp 76-79°. Assigned the (*R*)- config. Not interrelated with Unanisoflavan.

Gottleib, O.R. *et al*, *Phytochemistry*, 1975, **14**, 2495 (*deriv*)
Minhaj, N. *et al*, *Tetrahedron Lett.*, 1976, 2391 (*isol, struct*)

1,2-Undecadiene, 9CI U-80003

[56956-46-8]

$$H_3C(CH_2)_7CH{=}C{=}CH_2$$

$C_{11}H_{20}$ M 152.279

Liq. d_4^{22} 0.773. Bp_{13} 84-85°. n_D^{22} 1.4443.

Moreau, J.L. *et al*, *J. Organomet. Chem.*, 1976, **108**, 159 (*synth, ir, raman*)
Michelot, D. *et al*, *Tetrahedron Lett.*, 1976, 275 (*use*)
Buechi, G. *et al*, *J. Org. Chem.*, 1979, **44**, 4116 (*synth, ir, pmr*)
Hana, S. *et al*, *Chem. Lett.*, 1984, 345 (*use*)
Searles, S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1984, 747 (*synth, ir, pmr, ms*)
Colas, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1987, 165 (*synth, ir, raman*)

1,3-Undecadiene, 9CI U-80004

[54826-10-7]

$$H_2C{=}CHCH{=}CH(CH_2)_6CH_3$$

$C_{11}H_{20}$ M 152.279

(E)-form [79309-74-3]

Bp_{40} 135°.

Tsai, D.J.S. *et al*, *Tetrahedron Lett.*, 1981, **22**, 2751 (*synth, pmr*)
Jabri, N. *et al*, *Bull. Soc. Chim. Fr.*, *Part* 2, 1983, 321 (*synth, ir, pmr, cmr*)
Ishibashi, H. *et al*, *Tetrahedron Lett.*, 1985, **26**, 5791 (*synth*)
Yamada, S. *et al*, *J. Org. Chem.*, 1986, **51**, 4934 (*synth*)
Ishibashi, H. *et al*, *J. Chem. Res.* (*S*), 1987, 296 (*use*)

1,4-Undecadiene, 9CI U-80005

[53786-93-9]

$$H_3C(CH_2)_5CH{=}CHCH_2CH{=}CH_2$$

$C_{11}H_{20}$ M 152.279

Constituent of ginseng oil (*Panax ginseng*) and of Chinese traditional medicine, Gaoben (*Ligusticum* sp.).

(E)-form [55976-13-1]

$Bp_{0.2}$ 37-38°. n_D^{20} 1.4385.

(Z)-form [55976-14-2]

Used in synthetic flavour components. Bp_{10} 66-67°.

Lynd, R.A. *et al*, *Synthesis*, 1974, 658 (*synth*)
Eisch, J.J. *et al*, *J. Org. Chem.*, 1976, **41**, 2214 (*synth, ir, pmr*)
Uchida, K. *et al*, *J. Org. Chem.*, 1976, **41**, 2215 (*synth, ir, pmr, ms*)
Bosshardt, H. *et al*, *Helv. Chim. Acta*, 1980, **63**, 2393 (*synth, use, ir, pmr, ms*)
Kim, K.R. *et al*, *Chromatographia*, 1982, **15**, 559 (*ms*)
Hoshi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 2855 (*synth, pmr, ms, ir*)
Arase, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1984, **57**, 209 (*synth, use, pmr, ir*)

1,5-Undecadiene, 9CI U-80006

$$H_3C(CH_2)_4CH{=}CHCH_2CH_2CH{=}CH_2$$

$C_{11}H_{20}$ M 152.279

Liq. d_4^{20} 0.764. Bp_{10} 67°. n_D^{20} 1.4381. Mixt. of *E*- and *Z*-forms.

Prevost, C. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 2485 (*synth*)
Rossi, R. *et al*, *Tetrahedron Lett.*, 1986, **27**, 2529 (*synth*)

1,6-Undecadiene, 9CI U-80007

$$H_3C(CH_2)_3CH{=}CH(CH_2)_3CH{=}CH_2$$

$C_{11}H_{20}$ M 152.279

Liq. Bp_{10} 73-76°. Mixt. of *Z*- and *E*- isomers.

[71309-05-2, 91914-03-3]

Zakharkin, L.I. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1979, 1400; *CA*, **91**, 123342z (*synth*)
Barluenga, J. *et al*, *J. Chem. Res.* (*S*), 1984, 122 (*synth, ir, pmr*)

1,10-Undecadiene, 9CI U-80008

[13688-67-0]

$H_2C{=}CH(CH_2)_7CH{=}CH_2$

$C_{11}H_{20}$ M 152.279
Mobile liq. d_4^{20} 0.767. Bp_{756} 187°, Bp_{100} 120°. n_D^{20} 1.4352.

Casteignau, G. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 3893, 3904 (*synth, glc, struct*)
Shono, T. *et al*, *Chem. Lett.*, 1978, 69 (*synth*)
Reiner, E. *et al*, *Biomed. Mass Spectrom.*, 1979, **6**, 491 (*ms, glc*)
Cruz de Maldonado, V. *et al*, *Synth. Commun.*, 1983, **13**, 1163 (*synth*)

2,3-Undecadiene, 9CI U-80009

[57648-44-9]

$H_3CCH{=}C{=}CH(CH_2)_6CH_3$

$C_{11}H_{20}$ M 152.279

(±)-*form*
Liq. d_4^{22} 0.772. Bp_{11} 80°. n_D^{22} 1.4560.

Moreau, J.L. *et al*, *J. Organomet. Chem.*, 1976, **108**, 159 (*synth, ir*)
Barluenga, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 203 (*synth, ir, raman*)

2,4-Undecadiene, 9CI U-80010

[59742-41-5]

$H_3CCH{=}CHCH{=}CH(CH_2)_5CH_3$

$C_{11}H_{20}$ M 152.279

[66717-31-5, 66717-32-6, 66717-34-8, 66717-37-1]

Auclair, F. *et al*, *Bull. Soc. Chim. Fr.*, 1976, 142 (*synth, ir, uv, pmr*)
Dang, H.P. *et al*, *Tetrahedron Lett.*, 1978, 191 (*synth*)
Ukai, J. *et al*, *Tetrahedron Lett.*, 1984, **25**, 5173 (*synth*)
Herve du Penhoat, C. *et al*, *Tetrahedron*, 1986, **42**, 4807 (*synth, ms, pmr, ir*)
Umano, K. *et al*, *J. Agric. Food Chem.*, 1987, **35**, 14 (*glc*)
Ikeda, Y. *et al*, *Tetrahedron*, 1987, **43**, 731 (*synth, pmr*)
Cuvigny, T. *et al*, *Tetrahedron*, 1987, **43**, 859 (*synth*)

2,5-Undecadiene, 9CI U-80011

[76345-96-5]

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_3$

$C_{11}H_{20}$ M 152.279
Liq. Bp_{15} 67-73°. Mixt. of geom. isomers.

[72820-71-4]

Alexakis, A. *et al*, *Synthesis*, 1979, 826 (*synth, ir, pmr*)
Gaspanoli, A. *et al*, *Riv. Ital. Sostanze Grasse*, 1985, **62**, 91; *CA*, **103**, 140446v (*ms, glc*)

2,9-Undecadiene, 8CI U-80012

[22057-21-2]

$H_3CCH{=}CH(CH_2)_5CH{=}CHCH_3$

$C_{11}H_{20}$ M 152.279

Casteignau, G. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 3904 (*synth, ir, glc*)

3,5-Undecadiene, 9CI U-80013

$H_3CCH_2CH{=}CHCH{=}CH(CH_2)_4CH_3$

$C_{11}H_{20}$ M 152.279
Oil. $Bp_{0.01}$ 32°. Mixt. of stereoisomers.

[78500-37-5, 78500-38-6, 78500-39-7, 86593-86-4]

Jabri, N. *et al*, *Bull. Soc. Chim. Fr., Part II*, 1983, 332 (*synth, ir, pmr, cmr*)
Bloch, R. *et al*, *Tetrahedron Lett.*, 1983, **24**, 1247 (*synth*)
Einhorn, J. *et al*, *Tetrahedron Lett.*, 1985, **26**, 1445 (*ms*)

4,6-Undecadiene, 9CI U-80014

[50284-90-7]

$H_3C(CH_2)_3CH{=}CHCH{=}CHCH_2CH_2CH_3$

$C_{11}H_{20}$ M 152.279
Liq. Bp 46-48°. n_D^{26} 1.4618.

Negishi, E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 606 (*synth*)

4,7-Undecadiene, 9CI U-80015

[104645-53-6]

$H_3CCH_2CH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH_3$

$C_{11}H_{20}$ M 152.279

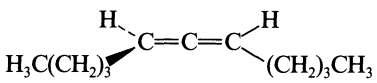
(*Z,Z*)-*form* [43040-05-7]
Bp_{16} 80-81.5°.

Clements, A.H. *et al*, *J. Am. Oil Chem. Soc.*, 1973, **50**, 325 (*synth, ir, pmr*)
Carless, H.A.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 1999 (*synth, pmr*)

5,6-Undecadiene, 9CI U-80016

1,3-Dibutylallene

[18937-82-1]



(*R*)-*form*

$C_{11}H_{20}$ M 152.279

(*R*)-*form* [65253-20-5]
$[\alpha]_D^{25}$ −33.4° (c, 7 in $CHCl_3$).

(*S*)-*form* [65253-19-2]
$[\alpha]_D^{25}$ −34.7° (c, 5 in $CHCl_3$).

(±)-*form* [111555-44-3]
Oil. Bp_{15} 70-80°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1967, **100**, 3706 (*synth, ms, ir, pmr*)
Wiensig, J.R. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 532 (*ms, synth*)
Pirkle, W.H. *et al*, *J. Org. Chem.*, 1978, **43**, 1950 (*synth*)
Kostikov, R.R. *et al*, *Zh. Prikl. Spektrosk.*, 1983, **39**, 486; *CA*, **99**, 186173f (*cmr*)
Fujisawa, T. *et al*, *Tetrahedron Lett.*, 1984, **25**, 4007 (*synth*)
Alexakis, A. *et al*, *Tetrahedron Lett.*, 1985, **26**, 4197 (*synth*)
Marek, I. *et al*, *Tetrahedron Lett.*, 1986, **27**, 5499 (*synth*)
Colas, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1987, 165 (*synth, ir, raman*)

1,3-Undecadien-5-yne, 9CI U-80017

$H_3C(CH_2)_4C{\equiv}CCH{=}CHCH{=}CH_2$

$C_{11}H_{16}$ M 148.247

(*E*)-*form* [56318-81-1]
Liq. $Bp_{2.5}$ 76-77°.

(*Z*)-*form* [56318-73-1]
Obt. by glc.

Näf, F. *et al*, *Helv. Chim. Acta*, 1975, **58**, 1016 (*synth, pmr, ms*)
Andreini, B.P. *et al*, *Tetrahedron*, 1987, **43**, 4591 (*synth, pmr, ir*)

1,5-Undecadien-3 yne U-80018

$H_3C(CH_2)_4CH{=}CHC{\equiv}CCH{=}CH_2$

$C_{11}H_{16}$ M 148.247

(E)-form
Liq. Bp_4 79-80°.

Andreini, B.P. *et al*, *Tetrahedron*, 1987, **43**, 4591 (*synth, pmr, ir, ms*)

4,7-Undecadiyne, 9CI U-80019

[115410-63-4]

$H_3CCH_2CH_2C{\equiv}CCH_2C{\equiv}CCH_2CH_2CH_3$

$C_{11}H_{16}$ M 148.247
Liq. Bp_5 74-82°.

Clements, A.H. *et al*, *J. Am. Oil Chem. Soc.*, 1973, **50**, 325 (*synth, ir*)
Carless, H.A.J. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1987, 1999 (*synth, ir, pmr, cmr*)

2,4-Undecadiyn-1-ol U-80020

$H_3C(CH_2)_5C{\equiv}CC{\equiv}CCH_2OH$

$C_{11}H_{16}O$ M 164.247
Oil.

Kerdesky, F.A.J. *et al*, *J. Med. Chem.*, 1987, **30**, 1177 (*synth, pmr*)

6-Undecen-1-ol U-80021

$H_3C(CH_2)_3CH{=}CH(CH_2)_4CH_2OH$

$C_{11}H_{22}O$ M 170.294

(E)-form [16695-37-7]
Liq. $Bp_{0.6}$ 84-85°.

(Z)-form [68760-60-1]
Liq. $Bp_{0.01}$ 78-80°.

Green, N. *et al*, *J. Med. Chem.*, 1967, **10**, 533.
Svirskaya, P.I. *et al*, *J. Chem. Eng. Data*, 1979, **24**, 152.
Brown, H.C. *et al*, *J. Org. Chem.*, 1988, **53**, 246 (*synth, ir, pmr, cmr*)

10-Undecen-2-one, 9CI U-80022

[36219-73-5]

$H_2C{=}CH(CH_2)_7COCH_3$

$C_{11}H_{20}O$ M 168.278
Constit. of *Pinus mugo* essential oil. Bp 235°.

Cottier, L. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 1072 (*synth*)
Bambagiotti, A.M. *et al*, *Planta Med.*, 1981, **43**, 39 (*isol*)
Ashby, E.C. *et al*, *Organometallics*, 1984, **3**, 1718 (*synth, pmr*)

5-Undecen-2-one U-80023

$H_3C(CH_2)_4CH{=}CHCH_2CH_2COCH_3$

$C_{11}H_{20}O$ M 168.278

(Z)-form [21944-96-7]
Pheromone from the pedal gland of the bontebok *Damaliscus dorcas dorcas*.

Yamashita, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3368 (*synth, pmr, bibl*)

1-Undecyn-5-ol, 9CI U-80024

[72957-73-4]

$H_3C(CH_2)_5CH(OH)CH_2CH_2C{\equiv}CH$

$C_{11}H_{20}O$ M 168.278

(±)-form
Oil. Bp_2 140°.

Subramaniam, C.S. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1979, 2346 (*synth, uv, pmr, use*)

3-Undecyn-1-ol, 9CI U-80025

[54299-09-1]

$H_3C(CH_2)_6C{\equiv}CCH_2CH_2OH$

$C_{11}H_{20}O$ M 168.278
Oil. $Bp_{0.25}$ 79-80°.

Holland, B.C. *et al*, *Chem. Phys. Lipids*, 1974, **13**, 239.
Gershon, H. *et al*, *J. Pharm. Sci.*, 1985, **74**, 556.

4-Undecyn-1-ol, 9CI U-80026

[54377-35-4]

$H_3C(CH_2)_5C{\equiv}CCH_2CH_2CH_2OH$

$C_{11}H_{20}O$ M 168.278
Oil. Bp_{20} 133-140°, $Bp_{0.03}$ 80°. n_D^{25} 1.4586.
4-Methylbenzensulfonyl: Thick oil.

Ames, D.E. *et al*, *J. Chem. Soc.*, 1963, 5889 (*synth*)
Lie Ken Jie, M.S.F. *et al*, *J. Chromatogr.*, 1974, **97**, 165 (*ester, synth, glc*)
Svirskaya, P.A. *et al*, *J. Chem. Eng. Data*, 1979, **24**, 152 (*synth, ir, pmr*)
Reddy, P.S. *et al*, *Synth. Commun.*, 1984, **14**, 327 (*synth, pmr*)
Vig, O.P. *et al*, *Indian J. Chem., Sect. B*, 1986, **25**, 1042 (*synth, ir, pmr*)
Kabalka, G.W. *et al*, *J. Org. Chem.*, 1986, **51**, 2386 (*deriv, synth, pmr, cmr*)

4-Undecyn-2-ol, 9CI U-80027

[95061-41-9]

$H_3C(CH_2)_5C{\equiv}CCH_2CH(OH)CH_3$

$C_{11}H_{20}O$ M 168.278
Oil. $Bp_{0.2}$ 65-72°.

Utimoto, K. *et al*, *Tetrahedron Lett.*, 1984, **25**, 5423 (*synth*)
Oehlschlager, A.C. *et al*, *Can. J. Chem.*, 1986, **64**, 1407 (*synth, use*)

5-Undecyn-1-ol, 9CI U-80028

[69222-09-9]

$H_3C(CH_2)_4C{\equiv}C(CH_2)_3CH_2OH$

$C_{11}H_{20}O$ M 168.278
Oil. $Bp_{0.01}$ 83-84°. n_D^{25} 1.4586.

Lie Ken Jie, M.S.F. *et al*, *J. Chromatogr.*, 1974, **97**, 152 (*synth, glc*)
Svirskaya, P.A. *et al*, *J. Chem. Eng. Data*, 1979, **24**, 152 (*synth*)

5-Undecyn-2-ol, 9CI U-80029

[92051-76-8]

$H_3C(CH_2)_4C{\equiv}CCH_2CH_2CH(OH)CH_3$

$C_{11}H_{20}O$ M 168.278

(±)-form
Oil. Bp_1 110°.

Reddy, P.S. *et al*, *Synth. Commun.*, 1984, **14**, 327 (*synth, pmr*)

6-Undecyn-5-ol, 9CI U-80030

[73252-74-1]

$H_3C(CH_2)_3C{\equiv}CCH(OH)(CH_2)_3CH_3$

$C_{11}H_{20}O$ M 168.278

(±)-*form* [111462-96-5]
Oil. Bp_1 65°.

Overman, L.E. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 747.
Colas, Y. *et al*, *Bull. Soc. Chim. Fr.*, 1987, 165 (*synth*, *ir*)

7-Undecyn-1-ol, 9CI U-80031

[69222-11-3]

$H_3CCH_2CH_2C{\equiv}C(CH_2)_5CH_2OH$

$C_{11}H_{20}O$ M 168.278
Oil. $Bp_{0.04}$ 84-86°. n_D^{24} 1.4600.

Svirskaya, P.A. *et al*, *J. Chem. Eng. Data*, 1979, **24**, 152 (*synth*, *use*, *ir*, *pmr*)

10-Undecyn-2-ol, 9CI U-80032

[104903-89-1]

$HC{\equiv}C(CH_2)_7CH(OH)CH_3$

$C_{11}H_{20}O$ M 168.278

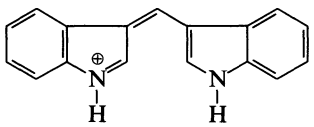
Me ether: 10-Methoxy-1-undecyne
$C_{12}H_{22}O$ M 182.305
Isol. from ethereal oil of *Litsea odorifera*. Oil. d^{20} 0.824. n_D^{20} 1.4400.

Mathews, W.J. *et al*, *Chem. Ind.* (*London*), 1963, 122 (*isol*, *deriv*)
Oehlschlager, A.C. *et al*, *Can. J. Chem.*, 1986, **64**, 1407 (*synth*, *use*)

Urorosein U-80033

(3H-Indol-3-ylidenemethyl)-1H-indole(1+), 9CI. 3-Indol-3-ylmethylene-3H-indol-3-ium. Di-3-indolylcarbenium

[526-32-9]



$C_{17}H_{13}N_2^{\oplus}$ M 245.303
Pigment.

Chloride:
$C_{17}H_{13}ClN_2$ M 280.756
Deep red needles ($EtOH/Me_2CO$).

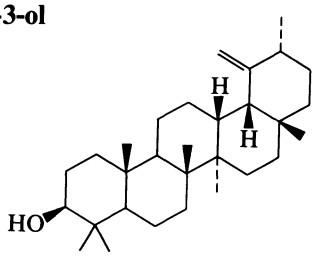
Bromide:
$C_{17}H_{13}BrN_2$ M 325.207
Deep red prisms (EtOH).

Perchlorate:
$C_{17}H_{13}ClN_2O_4$ M 344.753
Red cryst. with greenish metallic lustre. Carbonises without melting.

Tetrafluoroborate: [102652-01-7].
$C_{17}H_{13}BF_4N_2$ M 332.108
Orange-yellow cryst. Mp 225°.

Harley-Mason, J. *et al*, *Biochem. J.*, 1952, **51**, 430 (*synth*)
Smith, G.F., *J. Chem. Soc.*, 1954, 3842 (*synth*)
Mueller, J. *et al*, *Monatsh. Chem.*, 1985, **116**, 365 (*analogues*)
Pinder, U. *et al*, *Justus Liebigs Ann. Chem.*, 1986, 1621 (*synth*, *ir*, *uv*)

19(29)-Ursen-3-ol U-80034



$C_{30}H_{50}O$ M 426.724

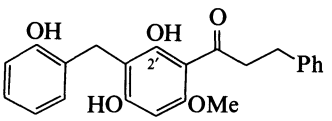
3β-form [117895-04-2] ***Calotropenol***
Needles ($CHCl_3/C_6H_6$). Mp 168°. $[\alpha]_D$ +37.26° (c, 0.161 in $CHCl_3$).

Ac: [118013-26-6]. *3β-Acetoxy-19(29)-ursene. Calotropenyl acetate*
$C_{32}H_{52}O_2$ M 468.762
Constit. of *Calotropis procera*. Cryst. Mp 198°. $[\alpha]_D$ +8.9° (c, 0.415 in $CHCl_3$).

Khan, A.Q. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 925.

Uvaretin U-80035

Updated Entry replacing U-50017
1-[2,4-Dihydroxy-3-[(2-hydroxyphenyl)methyl]-6-methoxyphenyl]-3-phenyl-1-propanone, 9CI. Chamuvarin
[58449-06-2]



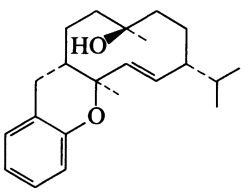
$C_{23}H_{22}O_5$ M 378.424
Isol. from *Uvaria acuminata*, *U. chamae* and *Croton californicus*. Cryst. (MeCN or C_6H_6). Mp 164-165°.

O-*De-Me*, 2′-O-*Me:* [61463-03-4]. ***Isouvaretin***
$C_{23}H_{22}O_5$ M 378.424
Constit. of *U. chamae* and *U. angolensis*. Cryst. ($CHCl_3$/hexane). Mp 80-82°.

Cole, J.R. *et al*, *J. Org. Chem.*, 1976, **41**, 1852 (*isol*, *struct*)
Lasswell, W.L. *et al*, *J. Org. Chem.*, 1977, **42**, 1295 (*isol*)
Tammani, B. *et al*, *Phytochemistry*, 1977, **16**, 2040 (*isol*)
Hufford, C.D. *et al*, *Phytochemistry*, 1980, **19**, 2036 (*isol*, *cmr*, *Uvaretin*, *Isouvaretin*)
Jain, A.C. *et al*, *Indian J. Chem.*, *Sect. B*, 1985, **24**, 1015 (*synth*)

Uvarisesquiterpene A U-80036

[117176-62-2]

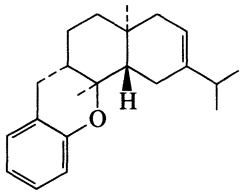


$C_{22}H_{32}O_2$ M 328.494
Constit. of *Uvaria angolensis*. Amorph. $[\alpha]_D$ −16° (c, 0.12 in $CHCl_3$).

Muhammad, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 719.

Uvarisesquiterpene B **U-80037**

[117176-79-1]



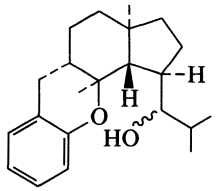
$C_{22}H_{30}O$ M 310.478

Constit. of *Uvaria angolensis*. Amorph.

Muhammad, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 719.

Uvarisesquiterpene C **U-80038**

[117176-80-4]



$C_{22}H_{32}O_2$ M 328.494

Constit. of *Uvaria angolensis*. Amorph.

Muhammad, I. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 719.

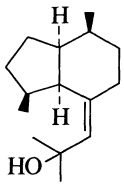
V

Valerenenol V-80001

Updated Entry replacing V-30001

*2-Methyl-1-(octahydro-3,7-dimethyl-4*H*-inden-1-ylidene)-2-propanol, 9CI*

[84249-43-4]



Absolute configuration

$C_{15}H_{26}O$ M 222.370

Constit. of soft coral *Xeniidae* sp. Oil. $[\alpha]_D$ +123° ($CHCl_3$).

(E)-*isomer:* [84249-42-3]. ***Isovalerenenol***

Constit. of *X.* sp. Semisolid. $[\alpha]_D$ +45° ($CHCl_3$).

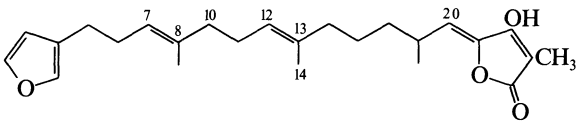
Kobayashi, M. *et al*, *Chem. Pharm. Bull.*, 1982, **30**, 3431 (*isol, pmr, cmr, cryst struct*)

Variabilin† V-80002

Updated Entry replacing V-70003

*5-[13-(3-Furanyl)-2,6,10-trimethyl-6,10-tridecadienylidene]-4-hydroxy-3-methyl-2(5*H*)-furanone, 9CI*

[51847-87-1]



$C_{25}H_{34}O_4$ M 398.541

Isol. from the sponge *Ircinia strobilina* and a *Sarcotragus* sp. Plant phytoalexin with antibiotic props. Oil. $[\alpha]_D$ −4° (c, 1 in $CHCl_3$). λ_{max} 255 nm (MeOH).

*20*E*-Isomer:* [114761-90-9].

$C_{25}H_{34}O_4$ M 398.541

Constit. of a *S.* sp. Oil.

Δ^{13}*-Isomer* (Z-)*:* [114728-09-5].

$C_{25}H_{34}O_4$ M 398.541

Constit. of a *S.* sp. Oil. $[\alpha]_D$ −4.4° (c, 0.9 in $CHCl_3$).

7,8-Dihydro, 8-hydroxy: [82124-11-6]. ***8-Hydroxyvariabilin***

$C_{25}H_{36}O_5$ M 416.556

Constit. of a *S.* sp. Oil. $[\alpha]_D$ −24.5° (c, 0.22 in MeOH).

5-Hydroxy: ***5-Hydroxyvariabilin***

$C_{25}H_{34}O_5$ M 414.541

Constit. of an *Ircinia* sp.

5-Oxo: ***5-Oxovariabilin***

$C_{25}H_{32}O_5$ M 412.525

Constit. of an *I.* sp.

5-Oxo, $\Delta^{8(10)}$*-isomer*(E-)*:* ***5-Oxo-8(10)*E*-variabilin***

$C_{25}H_{32}O_5$ M 412.525

Constit. of an *I.* sp.

5-Oxo, $\Delta^{8(10)}$(E-), Δ^{13}*-isomer:*

$C_{25}H_{32}O_5$ M 412.525

Constit. of an *I.* sp.

Faulkner, D.J., *Tetrahedron Lett.*, 1973, 3821 (*isol, uv, ir, nmr, struct*)

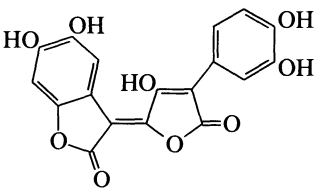
Rothberg, I. *et al*, *Tetrahedron Lett.*, 1975, 769 (*isol, ir, uv, nmr, struct*)

Barrow, C.J. *et al*, *J. Nat. Prod.* (*Lloydia*), 1988, **51**, 275, 1294 (*isol, deriv, pmr, cmr*)

Variegatorubin V-80003

*3-[4-(3,4-Dihydroxyphenyl)-3-hydroxy-5-oxo-2-(5*H*)furanylidene]-5,6-dihydroxy-2(3*H*)-benzofuranone, 9CI*

[27286-59-5]



$C_{18}H_{10}O_9$ M 370.272

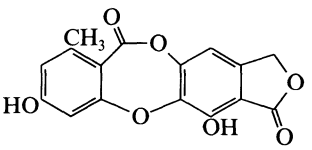
Isol. from *Suillus piperatus* and *Rhizopogon roseolus*. Brown-violet fine needles (MeCN). Mp >320° dec.

Steglich, W. *et al*, *Z. Naturforsch.*, *B*, 1970, **25**, 557; 1971, **26**, 376 (*isol, struct*)

Variolaric acid V-80004

*4,7-Dihydroxy-9-methyl-10*H*-isobenzofuro[5,6-b][1,4]benzodioxepin-3,10(1*H*)-dione, 9CI. Ochrolechic acid*

[490-34-6]



$C_{16}H_{10}O_7$ M 314.251

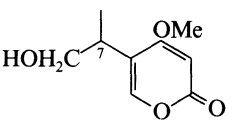
Lichen acid from *Lecanora rupicola*. Needles (MeOH). Mp 296° dec.

Devlin, J.P. *et al*, *J. Chem. Soc. C*, 1971, 1318 (*isol, pmr, bibl*)

Rana, N.M. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1975, 2992 (*struct, ms, bibl*)

Jongen, R. *et al*, *J. Chem. Soc., Perkin Trans.* 1, 1979, 2588 (*synth*)

Vertipyronol V-80005



$C_9H_{12}O_4$ M 184.191

Metab. of *Leptographium wageneri*. Oil. $[\alpha]_D$ −1.58° (c, 0.19 in $CHCl_3$).

7-Hydroxy: ***Vertipyronediol***

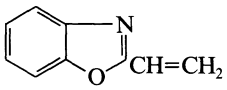
$C_9H_{12}O_5$ M 200.191

Metab. of *L. wageneri*. Cryst. (Me_2CO/hexane). Mp 128-129°. $[\alpha]_D$ −50° (c, 0.2 in $CHCl_3$).

Ayer, W.A. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 119 (*isol, ir, pmr, cmr*)

2-Vinylbenzoxazole V-80006

[63359-54-6]



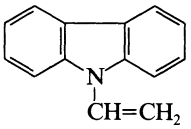
C_9H_7NO M 145.160
$Bp_{0.04}$ 75° (kugelrohr) .

Bartsch, H. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 795 (*synth*)

N-Vinylcarbazole V-80007

N-*Ethenylcarbazole*

[1484-13-5]



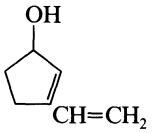
$C_{14}H_{11}N$ M 193.248
Important polymerisation monomer. Cryst. (EtOH). Mp 63.5-66°. Bp_{15} 175-178°, $Bp_{0.02}$ 68-70°.

Clemo, G.R. *et al*, *J. Chem. Soc.*, 1924, **125**, 1806 (*synth*)
Reppe, W. *et al*, *Justus Liebigs Ann. Chem.*, 1956, **601**, 81 (*synth*)
Takuze, S. *et al*, *Encycl. Polym. Sci. Technol.*, 1971, **14**, 281.

3-Vinyl-2-cyclopenten-1-ol V-80008

3-Ethenyl-2-cyclopenten-1-ol, 9CI

[114614-91-4]



$C_7H_{10}O$ M 110.155

(±)-***form***
Golden oil.

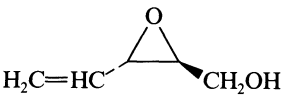
Me ether: 3-Methoxy-1-vinylcyclopentene
$C_8H_{12}O$ M 124.182
Liq. Bp_{66} 87-89°.

[114614-87-8]

Fisher, M.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 4625 (*synth, pmr, cmr, ir, ms*)

3-Vinyl-2-oxiranemethanol V-80009

3-Ethenyl-2-oxiranemethanol. 2,3-Epoxy-4-penten-1-ol



(2*S*,3*S*)-*form*

$C_5H_8O_2$ M 100.117

(2*S*,3*S*)-***form***
$Bp_{5.5}$ 67°. $[\alpha]_D^{23}$ −58.7° (neat). >91% enantiomeric excess.

O-(*4-Methylbenzenesulfonyl*): Solid. Mp 56.5-58°. $[\alpha]_D^{23}$ −33.3° (c, 0.96 in EtOH).

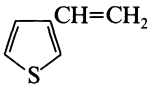
(±)-***form***
Bp_{18} 92°.

Wershofen, S. *et al*, *Synthesis*, 1988, 854 (*synth, ms, ir, pmr, cmr*)

3-Vinylthiophene V-80010

3-Ethenylthiophene, 9CI

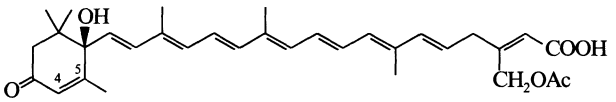
[13679-64-6]



C_6H_6S M 110.179
Liq. d_4^{15} 1.08. Bp 160°, Bp_{20} 55-59°.

Troyanowsky, C., *Bull. Soc. Chim. Fr.*, 1955, 424 (*synth*)
Tominaga, Y. *et al*, *J. Heterocycl. Chem.*, 1981, **18**, 967 (*synth, ir, pmr*)
Abarca, B. *et al*, *Tetrahedron*, 1987, **43**, 269 (*synth, props*)

Vitixanthin V-80011



$C_{33}H_{42}O_6$ M 534.691
Constit. of root of *Cochlospermum vitifolium*.

Me ester: $[\alpha]_D^{20}$ −558° ($CHCl_3$).

4,5-Dihydro: ***Dihydrovitixanthin***
$C_{33}H_{44}O_6$ M 536.707
Constit. of *C. vitifolium*.

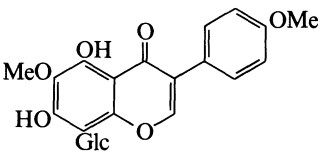
4,5-Dihydro, Me ester: $[\alpha]_D^{20}$ −82° ($CHCl_3$).

Achenbach, H. *et al*, *Tetrahedron Lett.*, 1989, **30**, 3059.

Volubilinin V-80012

8-β-D-Glucopyranosyl-5,7-dihydroxy-6-methoxy-3-(4-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI. 8-C-Glucosyl-5,7-dihydroxy-4′,6-dimethoxyisoflavone. Irisolidone 8-C-glucoside

[58930-58-8]



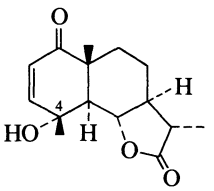
$C_{23}H_{24}O_{11}$ M 476.436
Isol. from flowers of *Dalbergia volubilis*. Plates (EtOAc/MeOH). Mp 159-161°.

Chawla, H.M. *et al*, *Phytochemistry*, 1976, **15**, 235.

Vulgarin V-80013

Updated Entry replacing V-60017
Tauremisin A. *Barrelin. Judaicin*

[3162-56-9]



Absolute configuration

$C_{15}H_{20}O_4$ M 264.321

Constit. of *Artemisia vulgaris*, *A. judaica* and *A. taurica*.
Oral hypoglycemic agent. Cryst. (EtOH). Mp 174-175°. $[\alpha]^{27}_{546}$ +48.7° (c, 3.86 in $CHCl_3$).

▷ LE3170000.

4-Epimer: [66289-87-0]. ***4-Epivulgarin***
$C_{15}H_{20}O_4$ M 264.321
From *A. judaica* and *A. canariensis*. Cryst. (C_6H_6/hexane)(also descr. as gum). Mp 192-194°. $[\alpha]_D$ +77.5° (c, 5.7 in $CHCl_3$).

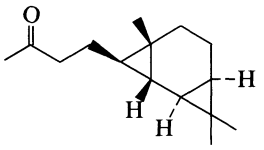
4-Deoxy,4α-hydroperoxy: [72505-77-2]. ***4α-Hydroperoxydesoxyvulgarin.*** *Peroxyvulgarin*
$C_{15}H_{20}O_5$ M 280.320
From *A. judaica*. Gum, needles (Me_2CO/Et_2O). Mp 170-171°. $[\alpha]_D$ −44° (c, 0.1 in MeOH).

[5091-07-6, 66289-87-0]

Geissman, T.A. *et al*, *J. Org. Chem.*, 1962, **27**, 1855 (*isol*, *struct*)
Ando, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1978, **51**, 283 (*synth*)
González, G. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1978, 1243 (*synth*)
Ando, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 2737 (*synth*)
Gonzalez, A.G. *et al*, *Phytochemistry*, 1983, **22**, 1509 (*isol*)
Metwally, M.A. *et al*, *Phytochemistry*, 1985, **24**, 1103 (*derivs*)
Abagaz, B. *et al*, *Tetrahedron*, 1986, **42**, 6003 (*cryst struct*)
Arias, J.M. *et al*, *J. Chem. Soc.*, *Perkin Trans.* 1, 1987, 471 (*synth*)
Al-Said, M.S. *et al*, *Phytochemistry*, 1989, **28**, 107 (*synth*)

W

Waitziacuminone W-80001



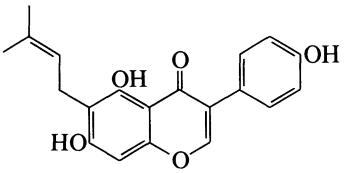
$C_{15}H_{24}O$ M 220.354
Constit. of *Waitzia acuminata*. Oil.

Jakupovic, J. *et al*, *Phytochemistry*, 1989, **28**, 1943.

Wighteone W-80002

5,7-Dihydroxy-3-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-6-prenyisoflavone. 6-Isopentenylgenistein. Erythrinin B

[51225-30-0]



$C_{20}H_{18}O_5$ M 338.359
Isol. from *Argyrocytisus battandieri*, *Erythrina variegata*, *Laburnum anagyroides*, *Lupinus albus*, *L. angustifolius*, *L. polyphyllus* and *Neonotonia wightii*. Phytoalexin. Bright-yellow plates (Me_2CO/C_6H_6). Mp 220-221°.

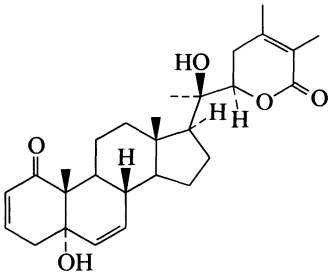
Tri-Ac: Cryst. (MeOH). Mp 160-162°.

Deshpande, V.H. *et al*, *Indian J. Chem.*, *Sect. B*, 1977, **15**, 205 (*isol*, *uv*, *pmr*, *struct*)
Ingham, J.L. *et al*, *Phytochemistry*, 1977, **16**, 1943 (*isol*, *ir*, *ms*, *struct*)

Withacoagin W-80003

5α,20-Dihydroxy-1-oxo-20R,22R-witha-2,6,24-trienolide

[119539-81-0]

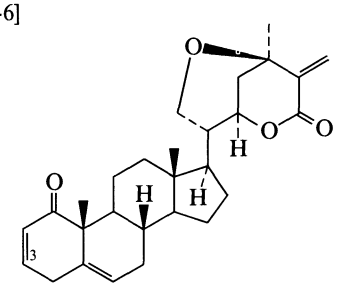


$C_{28}H_{38}O_5$ M 454.605
Constit. of *Withania coagulans*. Cryst. ($CHCl_3$). Mp 230-232°. $[\alpha]_D^{24}$ +114° (c, 0.19 in $CHCl_3$).

Neogi, P. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 4479.

Withametelin W-80004

[113430-43-6]



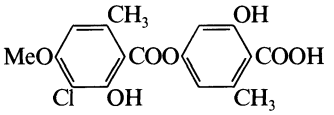
$C_{28}H_{36}O_4$ M 436.590
Constit. of leaves of *Datura metel*. Needles (EtOAc). Mp 210°. $[\alpha]_D$ −64.4° (c, 0.45 in $CHCl_3$).

Δ^3-*Isomer:* [123522-98-5]. ***Isowithametelin***
$C_{28}H_{36}O_4$ M 436.590
Constit. of *D. metel*. Cryst. Mp 280°. $[\alpha]_D$ −77.7° (c, 0.26 in $CHCl_3$).

Sinha, S.C. *et al*, *Tetrahedron*, 1989, **45**, 2165.

Wrightiin W-80005

[107783-44-8]



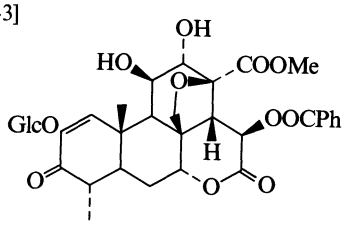
$C_{18}H_{17}ClO_7$ M 380.781
Constit. of *Erioderma wrightii*. Cryst. (EtOAc). Mp 216.5°.

Maass, W.S.G. *et al*, *Z. Naturforsch.*, *B*, 1986, **41**, 1589 (*isol*, *cryst struct*)
Elix, J.A. *et al*, *Aust. J. Chem.*, 1988, **41**, 1789 (*synth*)

Y

Yadanzioside M **Y-80001**

[101559-99-3]



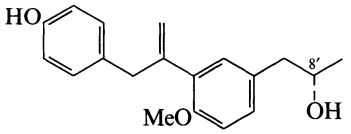
$C_{34}H_{40}O_{16}$ M 704.680

Constit. of *Brucea antidysenterica*. Amorph. powder. Mp 208-213°. $[\alpha]_D^{23}$ +39° (c, 0.41 in MeOH).

Okano, M. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 398 (*isol*)

Z

Zapotecol **Z-80001**

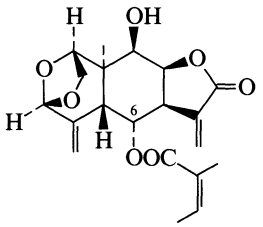


$C_{19}H_{22}O_3$ M 298.381
Constit. of *Krameria lanceolata*. Oil. $[\alpha]_D^{21}$ +5° (c, 0.6 in MeOH).

8′-Ketone: ***Zapotecone***
$C_{19}H_{20}O_3$ M 296.365
Constit. of *K. lanceolata*. Oil.

Achenbach, H. *et al*, *Phytochemistry*, 1989, **28**, 1959.

Zinaflorin IV **Z-80002**



$C_{20}H_{24}O_7$ M 376.405
Also represented in the ring opened form with epoxide and —CHO functions in ring A. Constit. of *Zinnia peruviana*. Cryst. Mp 194-196°. $[\alpha]_D$ +137.5° (c, 0.145 in $CHCl_3$), $[\alpha]_D$ +96.2° (c, 5.1 in EtOH).

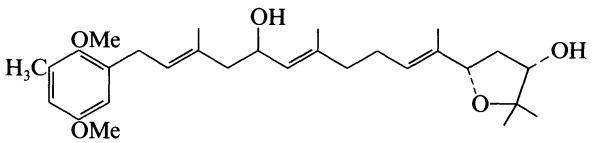
O^6*-Deacyl*, O^6*-tigloyl:* [88930-59-0].
$C_{20}H_{24}O_7$ M 376.405
Constit. of *Z. peruviana*.

O^6*-Deacyl*, O^6*-(2-methylpropenoyl):* [88930-72-7].
$C_{19}H_{22}O_7$ M 362.379
Constit. of *Z. peruviana*.

Herz, W. *et al*, *Phytochemistry*, 1981, **21**, 2229 (*isol*)
Ortega, A. *et al*, *Chem. Lett.*, 1983, 1607 (*cryst struct*)
Mirand, R. *et al*, *J. Nat. Prod.* (*Lloydia*), 1989, **52**, 1128 (*isol*, *pmr*)

Zosterdiol A **Z-80003**

[120163-23-7]

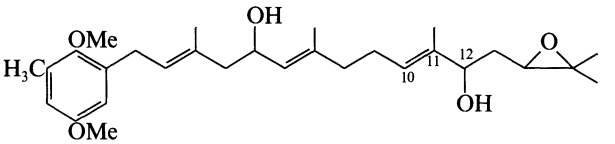


$C_{29}H_{44}O_5$ M 472.664
Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +0.5° (c, 2 in EtOH).

Amico, V. *et al*, *Phytochemistry*, 1989, **28**, 215.

Zosterdiol B **Z-80004**

[120163-24-8]



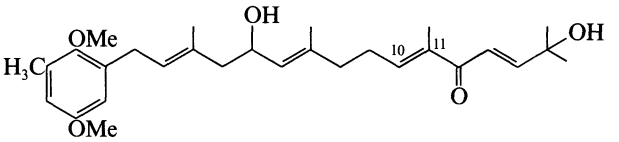
$C_{29}H_{44}O_5$ M 472.664
Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +1.1° (c, 0.9 in EtOH).

10,11-Dihydro 12-ketone: [120163-25-9]. ***Zosteronol***
$C_{29}H_{44}O_5$ M 472.664
Constit. of *C. zosteroides*. Oil. $[\alpha]_D^{20}$ +1.5° (c, 0.6 in EtOH).

Amico, V. *et al*, *Phytochemistry*, 1989, **28**, 215.

Zosterondiol B **Z-80005**

[120181-10-4]



$C_{29}H_{42}O_5$ M 470.648
Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +0.9° (c, 0.4 in EtOH).

10,11-Dihydro: [120181-09-1]. ***Zosterondiol A***
$C_{29}H_{44}O_5$ M 472.664
Constit. of *C. zosteroides*. Oil. $[\alpha]_D^{20}$ +0.7° (c, 0.8 in EtOH).

Amico, V. *et al*, *Phytochemistry*, 1989, **28**, 215.

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24-Acetoxy-12-deacetyl-12-epideoxoscalarin, A-80014
9β-Acetoxy-4,5-dehydro-4(15)-dihydrocostic acid, *in* H-60135
2-Acetoxy-2-desoxyperezone, *in* I-70075
4-Acetoxy-2,6-dibromo-1,5-dihydroxy-2-cyclohexen-1-one, *in* D-60097
6-Acetoxy-3,10-dibromo-4,7-epoxy-12-pentadecen-1-yne, *in* B-70217
4-Acetoxy-2,6-dibromo-5-hydroxy-2-cyclohexen-1-one, *in* D-60097
21-Acetoxy-21,23:24,25-diepoxyapotirucall-14-ene-3,7-diol, *in* T-60223
2α-Acetoxy-11α,13-dihydroconfertin, *in* D-60211
7α-Acetoxy-12,20-dihydroxy-8,12-abietadiene-11,14-dione, *in* R-60015
2′-Acetoxy-3,5-dihydroxy-7,8-dimethoxyflavone, *in* P-60045
12-Acetoxy-5,8-dihydroxyfarnesol, *in* T-60363
ent-3α-Acetoxy-1β,11α-dihydroxy-16-kaurene-6,15-dione, *in* T-80313
ent-12β-Acetoxy-7β,14α-dihydroxy-16-kaurene-3,15-dione, *in* T-80315
ent-1β-Acetoxy-7β,14α-dihydroxy-16-kaurene-3,15-dione, *in* T-80314
ent-14*S*-Acetoxy-1β,7β-dihydroxy-16-kauren-15-one, *in* T-50476
ent-7β-Acetoxy-1β,14*S*-dihydroxy-16-kauren-15-one, *in* T-50476
22*S*-Acetoxy-3α,15α-dihydroxy-7,9(11),24-lanostatren-26-oic acid, *in* T-80318
3α-Acetoxy-15α,22*S*-dihydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
22*S*-Acetoxy-3β,15α-dihydroxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318
2′-Acetoxy-5,5′-dihydroxy-3,7,8-trimethoxyflavone, *in* H-70080
20-Acetoxy-2β,3α-dihydroxy-1(15),8(19)-trinervitadiene, *in* T-70299
8-Acetoxy-2,6-dimethyl-3,6-octadien-2-ol, *in* D-80457

6-Acetoxy-3,7-dolabelladiene-12,16-diol, *in* D-70541
3β-Acetoxydrimenin, *in* D-60519
2α-Acetoxy-8-epiivangustin, *in* I-70109
6α-Acetoxy-8-epiivangustin, *in* I-70109
7β-Acetoxy-8α,13*R*-epoxy-6β,9α-dihydroxy-14-labden-11-one, *in* E-80037
6β-Acetoxy-1α,4α-epoxyeudesmane, *in* E-60019
4-Acetoxy-8,9-epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-ene, *in* M-80202
6-Acetoxy-3,4-epoxy-12-hydroxy-7-dolabellen-16-al, *in* D-70541
19-Acetoxy-15,16-epoxy-13,17-spatadien-5α-ol, *in* E-60029
ent-19-Acetoxy-7β,20-epoxy-1α,3α,6α,7α-tetrahydroxy-16-kauren-15-one, *see* M-80007
3β-Acetoxy-21,23-epoxy-7,24-tirucalladiene, *in* E-60032
3β-Acetoxy-10α-ethoxy-4,11(13)-cadinadien-12-oic acid, *in* Z-70001
9β-Acetoxy-4,11(13)-eudesmadien-12-oic acid, *in* H-60135
3β-Acetoxy-4,11(13)-eudesmadien-12,8β-olide, *in* H-60136
1β-Acetoxy-3,7(11),8-eudesmatrien-12,8-olide, *in* H-60140
1β-Acetoxy-4(15),7(11),8-eudesmatrien-12,8-olide, *in* H-60141
6β-Acetoxy-4(15)-eudesmene-1β,5α-diol, *in* E-60068
Acetoxyeumaitenol, *in* E-60072
4-Acetoxyflexilin, *in* F-70012
30-Acetoxy-3β-friedelanol, *in* F-80083
3β-Acetoxy-30-friedelanol, *in* F-80083
6α-Acetoxygedunin, *in* G-70006
11β-Acetoxygedunin, *in* G-70006
3-Acetoxy-1(10),5-germacradien-4-ol, *in* G-80010
17-Acetoxygutiesolbriolide, *in* G-80045
3β-Acetoxyhaageanolide acetate, *in* H-60001
2α-Acetoxyhardwickiic acid, *in* H-70002
5-*epi*-6β-Acetoxyhebemacrophyllide, *in* H-60010
6β-Acetoxyhebemacrophyllide, *in* H-60010
1-Acetoxy-6,8,12,14-hexadecatetraen-10-yne, *in* H-80041
8-Acetoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene, *in* H-70042
8-Acetoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-3-ene, *in* H-80047
15-Acetoxy-3α-hydroperoxyalloalantolactone, *in* A-80044
1-Acetoxy-7-hydroperoxy-3,7-dimethyl-2*E*,5*E*-octadien-4-one, *in* D-60318
3β-Acetoxy-10α-hydroxy-4,11(13)-cadinadien-12-oic acid, *in* Z-70001
ent-2α-Acetoxy-7β-hydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
ent-7β-Acetoxy-2α-hydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
1-Acetoxy-7-hydroxy-3,7-dimethyl-2*E*,5*E*-octadien-4-one, *in* D-60318
1β-Acetoxy-8β-hydroxy-3,7(11)-eudesmadien-12,8-olide, *in* D-60322
19-Acetoxy-18-hydroxygeranylnerol, *in* B-80151
6α-Acetoxy-2α-hydroxy-1(10),4,11(13)-germacratrien-12,8-olide, *in* H-70134
3β-Acetoxy-2α-hydroxy-1(10),4,11(13)-germacratrien-12,6α-olide, *in* H-60006
6β-Acetoxy-1β-hydroxy-4,11-guaiadien-3-one, *in* G-80044
8β-Acetoxy-10β-hydroxyhirsutinolide 13-*O*-acetate, *in* H-80089
8β-Acetoxy-10β-hydroxyhirsutinolide 1,13-*O*-diacetate, *in* H-80089
ent-14α-Acetoxy-7β-hydroxy-1,16-kauradiene-3,15-dione, *in* D-80324
ent-7β-Acetoxy-14α-hydroxy-1,16-kauradiene-3,15-dione, *in* D-80324
ent-3α-Acetoxy-11α-hydroxy-16-kaurene-6,15-dione, *in* D-80325
15α-Acetoxy-3α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314
3α-Acetoxy-15α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314
9α-Acetoxy-7β-hydroxy-2-longipinen-1-one, *in* D-80332
23-Acetoxy-30-hydroxy-20(29)-lupen-3-one, *in* D-70318
22-Acetoxy-3α-hydroxy-7α-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60328
3α-Acetoxy-15α-hydroxy-22-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60327
4-Acetoxy-6-(4-hydroxy-4-methyl-2-cyclohexenyl)-2-(4-methyl-3-pentenyl)-2-heptenoic acid, A-60018
2-(1-Acetoxy-4-hydroxy-4-methylpentyl)-5,8-dihydroxy-1,4-naphthoquinone, *in* D-80343
14-Acetoxy-9β-hydroxy-8β-(2-methylpropanoyloxy)-1(10),4,11(13)-germacratrien-12,6α-olide, *in* T-60323
6α-Acetoxy-17β-hydroxy-15,17-oxido-16-spongianone, *in* D-60365
15α-Acetoxy-3α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70330
3α-Acetoxy-15α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70330
3α-Acetoxy-15β-hydroxy-7,16-seco-7,11-trinervitadiene, *see* S-60019
3β-Acetoxy-19-hydroxy-13(16),14-spongiadien-2-one, *in* D-70345
15-Acetoxyisoalloalantolactone, *in* I-80047
17-Acetoxyisogutiesolbriolide, *in* I-80062
ent-17-Acetoxy-9β*H*-isopimara-7,15-diene, *in* I-80075
12β-Acetoxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
2-Acetoxyisopropenyl-6-acetyl-5-hydroxybenzofuran, *see* A-60065
ent-3β-Acetoxy-16β,17-kauranediol, *in* K-60005
3-Acetoxykaurenic acid, *in* H-80181
ent-1α-Acetoxy-16-kauren-19-oic acid, *in* H-80179
ent-3β-Acetoxy-15-kauren-17-oic acid, *in* H-60167
ent-3β-Acetoxy-16-kauren-18-oic acid, *in* H-80181
ent-3β-Acetoxy-15-kauren-17-ol, *in* K-60007
2β-Acetoxy-8(17),13*E*-labdadien-15-oic acid, *in* H-70147
2β-Acetoxy-8(17),13*Z*-labdadien-15-oic acid, *in* H-70147
ent-15-Acetoxy-7,13-labdadien-2α-ol, *in* L-80003
ent-15-Acetoxy-7,13-labdadien-2β-ol, *in* L-80004
ent-6β-Acetoxy-7,12*E*,14-labdatrien-17-oic acid, *in* L-60004
ent-6β-Acetoxy-7,12*E*,14-labdatrien-17-ol, *in* L-60004
15-Acetoxy-7-labden-17-oic acid, *in* H-60168
22-Acetoxy-8,23-lanostadiene-3α,25-diol, *in* L-80019
2α-Acetoxylaurenobiolide, *in* H-70134
3β-Acetoxy-14(26),17*E*,21-malabaricatriene, *in* M-60008
19-Acetoxymanoyl oxide, *in* E-70023
1-Acetoxy-6-(2-methoxy-4,5-methylenedioxyphenyl)-2-(3,4-methylenedioxyphenoxy)-3,7-dioxabicyclo[3.3.0]octane, *see* P-80140
3-Acetoxy-6-methoxyprimnatrienone, *in* P-80174
▷ 2-Acetoxy-1-methoxypropane, *in* P-70118
5-Acetoxymethyl-5′-(3-buten-1-ynyl)-2,2′-bithienyl, *in* B-80279
16β-Acetoxy-24-methyl-12,24-dioxo-25-scalaranal, *in* H-80200
3-Acetoxy-2-methyl-4(1*H*)-pyridinone, *in* H-80214
1*R*-Acetoxy-3-myodesertene, *in* M-80203
1*S*-Acetoxy-3-myodesertene, *in* M-80203
Acetoxyodontoschismenol, *in* D-70541
3β-Acetoxy-12-oleanene-2α,11α-diol, *in* O-60037
3β-Acetoxy-12-oleanene-1β,2α,11α-triol, *in* O-60034
3β-Acetoxy-28,13β-oleanolide, *in* H-60200
3β-Acetoxy-4,10(14)-oplopadiene-8β,9α-diol, *in* O-70042
2β-Acetoxy-3(14),8(10)-oplopadiene-6β,7α-diol (incorr.), *in* O-70042
ent-2α-Acetoxy-7-oxo-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
9β-Acetoxy-3-oxo-1,4(15),11(13)-eudesmatrien-12,6-olide, *in* H-60202
23-Acetoxy-3-oxo-20(30)-lupen-29-al, *in* D-70316
1-Acetoxy-4-[5-(1,3-pentadiynyl)-2-thienyl]-3-butyne, *in* P-80025
2-(1-Acetoxy-3-penten-1-ynyl)-5-(3-buten-1-ynyl)thiophene, *in* B-80281
1-Acetoxy-7-phenyl-2,4,6-heptatriyne, *in* P-80101
7-(3-Acetoxyphenyl)-2-heptene-4,6-diyn-1-ol, *in* H-80234
19-Acetoxy-9,(11),15-pimaradiene, *in* P-80148
1-Acetoxypinoresinol, *in* H-60221
1-Acetoxypinoresinol 4′-*O*-β-D-glucopyranoside, *in* H-60221
▷ 3-Acetoxy-1,2-propanediol, *see* G-60029
6β-Acetoxypulchellin 4-*O*-angelate, *in* P-80189
4-Acetoxy-10-puteninone, *see* L-60009
7α-Acetoxyroyleanone, *in* D-80265
12β-Acetoxysandaracopimaric acid, *in* S-80008
3′-Acetoxy-4′-senecioyloxy-3′,4′-dihydroseselin, *in* K-70013
12-Acetoxysesquisabinene, *in* S-70037
13-Acetoxysesquisabinene, *in* S-70037
3-Acetoxysterpurene, *in* S-80045
14-Acetoxy-8,10-tetradecadiene-4,6-diyn-3-ol, *in* T-80026
14-Acetoxy-2,4,8,10-tetradecaen-6-yne, *in* T-80031
13-Acetoxy-9-tetradecene-2,4,6-triyne, *in* T-80042
14-Acetoxytetraneurin *D*, *in* T-60158
1-Acetoxy-9-(2-thienyl)-4,6-nonadien-8-yne, *in* T-80181
3-Acetoxythiophene, *in* T-60212
17-Acetoxythymifodioic acid, *in* T-60218
9β-Acetoxytournefortiolide, *in* H-60137
9-Acetoxy-3,10,13-tribromo-4,7:6,12-diepoxy-1-pentadecyne, *in* B-70195
1-Acetoxy-2,12-tridecadiene-4,6,8,10-tetrayne, *in* T-80253
1-Acetoxy-2,8,10,12-tridecatetraene-4,6-diyne, *in* T-80260
8α-Acetoxy-3α,4α,10β-trihydroxy-1-guaien-12,6α-olide, *in* T-80094
ent-3α-Acetoxy-2α,6β,11β-trihydroxy-16-kauren-15-one, *in* P-80047
8-Acetoxy-2′,3,5-trihydroxy-7-methoxyflavone, *in* P-70029
15α-Acetoxy-5α,6β,14α-trihydroxy-1-oxo-20*S*,22*R*-witha-2,16,24-trienolide, *see* W-60006
16α-Acetoxy-2α,3β,12β-trihydroxy-4,7-pregnadien-20-one, *in* T-60124
15-Acetoxytubipofuran, *in* T-70332
3β-Acetoxy-28,20β-ursanolide, *in* H-60233
3β-Acetoxy-19(29)-ursene, *in* U-80034
3β-Acetoxy-12-ursene-2α,11α-diol, *in* U-60008
3β-Acetoxy-12-ursene-1β,2α,11α,20β-tetrol, *in* U-60005
3β-Acetoxy-12-ursene-2α,11α,20β-triol, *in* U-60007
3β-Acetoxy-12-ursene-1β,2α,11α-triol, *in* U-60006
3β-Acetoxywedeliasecokaurenolide, *in* W-60004
▷ Acetylacetone, *see* P-60059
Acetylacetone-thiourea, *see* D-60450

▷ 3-Acetylacrylic acid, *see* O-70098
Acetylaleuritolic acid, *in* H-80256
2-Acetyl-3-aminobenzofuran, A-70021
2-Acetyl-3-aminopyridine, A-70022
2-Acetyl-5-aminopyridine, A-70023
3-Acetyl-2-aminopyridine, A-70024
3-Acetyl-4-aminopyridine, A-70025
4-Acetyl-2-aminopyridine, A-70026
4-Acetyl-3-aminopyridine, A-70027
5-Acetyl-2-aminopyridine, A-70028
6-Acetyl-2-amino-1,7,8,9-tetrahydro-4*H*-pyrimido[4,5-*b*][1,4]diazepin-4-one, *see* A-70043
2-Acetyl-3-aminothiophene, A-70029
▷ Acetylandromedol, *in* G-80039
1-Acetylanthracene, A-70030
2-Acetylanthracene, A-70031
6-*O*-Acetylarbutin, *in* A-70248
[3][14-Acetyl-14-azacyclohexacosanone][25,26,53,54,55,56-hexaacetoxytricyclo[49.3.1.1^{24,28}]hexapentaconta-1(55),24,26,28(56),51,53-hexaene][14-acetyl-14-azacyclohexacosanone]catenane, A-60020
1-Acetyl-2-azidobenzene, *see* A-60334
1-Acetyl-3-azidobenzene, *see* A-60335
1-Acetyl-4-azidobenzene, *see* A-60336
Acetylbarlerin, *in* S-60028
p-Acetylbenzenethiol, *see* M-60017
2-Acetylbenzoic acid, A-80015
2-Acetyl-4*H*-1-benzopyran-4-one, A-80016
3-Acetyl-4*H*-1-benzopyran-4-one, A-80017
1-Acetylbiphenylene, A-80018
2-Acetylbiphenylene, A-80019
O-Acetyl-*N*-(4-biphenylyl)hydroxylamine, *see* A-80013
1-Acetyl-3-bromonaphthalene, A-60021
1-Acetyl-4-bromonaphthalene, A-60022
1-Acetyl-5-bromonaphthalene, A-60023
1-Acetyl-7-bromonaphthalene, A-60024
2-Acetyl-6-bromonaphthalene, A-60025
25-*O*-Acetylbryoamaride, *in* C-70204
2-Acetylbutadiene, *see* M-70075
Acetylbutadiyne, *see* H-60041
2-Acetylbutane, *see* M-70105
Acetyl-*tert*-butylcarbinol, *see* H-80154
γ-Acetylbutyraldehyde, *see* O-70091
O-Acetylcapillol, *in* P-80104
Acetylcedrene, A-70032
2-Acetyl-5-chloropyridine, A-70033
3-Acetyl-2-chloropyridine, A-70034
4-Acetyl-2-chloropyridine, A-70035
4-Acetyl-3-chloropyridine, A-70036
5-Acetyl-2-chloropyridine, A-70037
2-Acetylchromone, *see* A-80016
3-Acetylchromone, *see* A-80017
α-Acetylconstictic acid, *in* C-60163
1-Acetylcycloheptene, A-60026
1-Acetylcyclohexene, A-70038
4-Acetylcyclohexene, A-70039
1-Acetylcyclooctene, A-60027
1-Acetylcyclopentene, A-60028
6″-*O*-Acetyldaidzin, *in* D-80323
7-*O*-Acetyldaphnoretin, *in* D-70006
19-*O*-Acetyl-1,2-dehydrohautriwaic acid, *in* H-70002
3-Acetyl-2-desacetyl-22-epihippurin 1, *in* E-80039
4-Acetyl-2,3-dihydro-5-hydroxy-2-isopropenylbenzofuran, A-70040
N-Acetyl-*S*-[(5,8-dihydro-1-hydroxy-3-methoxy-7-methyl-5,8-dioxo-2-naphthalenyl)methyl]-L-cysteine, *in* F-70008
1-Acetyl-1,2-dihydro-3*H*-pyrrol-3-one, *in* D-70262
2-Acetyl-4,5-dihydrothiazole, A-70041
7-Acetyl-6,8-dihydroxy-3-methoxy-4,4-dimethyl-1(4*H*)-naphthalenone, A-80020
6-Acetyl-7,8-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran, *in* A-80023
5-Acetyl-2,2-dimethyl-1,3-dioxane-4,6-dione, A-60029
4-Acetyl-2,2-dimethyl-1,3-dioxolane, A-70042
3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one, *in* A-80021
3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-4-hydroxy-5,6-dimethyl-2*H*-pyran-2-one, A-80021
3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-4-hydroxy-5-methyl-6-propyl-2*H*-pyran-2-one, *in* A-80021
Acetyldinitromethane, *see* D-70454
Acetylenedicarboxaldehyde, *see* B-60351
Acetylenediurene, *see* T-70066
3-Acetyl-22-epihippurin-1, *in* E-80039
6-Acetylferulidin, *in* F-70006
5-*O*-(6-Acetyl-β-D-galactopyranosyl)-3′,4′-dihydroxy-7-methoxyneoflavone, *in* D-80356
6″-*O*-Acetylgenistin, *in* T-80309
6-Acetylhomopterin, A-70043
7-Acetylhorminone, *in* D-80265
5-Acetyl-2-hydroxybenzaldehyde, A-80022
3-Acetyl-4-hydroxy-2(5*H*)-furanone, A-60030
6-Acetyl-5-hydroxy-2-hydroxymethyl-2-methylchromene, A-60031
6-Acetyl-5-hydroxy-2-(1-hydroxymethylvinyl)benzo[*b*]furan, *in* A-60065
6-Acetyl-5-hydroxy-2-isopropenylbenzo[*b*]furan, *in* A-60065
5-Acetyl-2-(2-hydroxyisopropyl)benzofuran, *see* A-70044
6-Acetyl-7-hydroxy-8-methoxy-2,2-dimethyl-2*H*-1-benzopyran, A-80023
5-Acetyl-2-(1-hydroxy-1-methylethyl)benzofuran, A-70044
3-Acetyl-5-(hydroxymethyl)-7-hydroxy-2H-1-benzopyran-2-one, *see* A-80169
3-Acetyl-5-hydroxymethyl-7-hydroxycoumarin, *see* A-80169
▷ 4-Acetyl-2-hydroxy-3-methyltetrahydrofuran, *see* B-60194
2-Acetyl-3-hydroxy-5-(1-propynyl)thiophene, A-80024
Acetylimbricatolal, *in* H-70150
2-Acetyl-1*H*-indene, A-70045
3-Acetyl-1*H*-indene, A-70046
6-Acetyl-1*H*-indene, A-70047
1-Acetylindene, *see* A-70046
2-Acetylindole, A-60032
4-Acetylindole, A-60033
▷ 5-Acetylindole, A-60034
6-Acetylindole, A-60035
7-Acetylindole, A-60036
1-Acetyl-7-iodonaphthalene, A-60037
1-Acetyl-8-iodonaphthalene, A-60038
Acetylisomontanolide, *in* M-70154
1-Acetyl-4-isopentenyl-6-methylphloroglucinol, *in* T-70248
1-Acetyl-4-isopropenylcyclopentene, A-80025
4-Acetyl-2-isopropenyl-2,3-dihydro-5-benzofuranol, *see* A-70040
2-Acetyl-1-isopropylcyclopropaneacetic acid, *see* S-70027
1-Acetyl-4-isopropylidenecyclopentene, A-80026
1-Acetylisoquinoline, A-60039
3-Acetylisoquinoline, A-60040
4-Acetylisoquinoline, A-60041
5-Acetylisoquinoline, A-60042
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▷ 2-Amino-3-chloro-1,4-naphthalenedione, *see* A-70122
▷ 2-Amino-3-chloro-1,4-naphthoquinone, A-70122
3-Amino-2-chloro-1-propene, *see* C-70151
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2-Amino-8-chloro-9-β-D-ribofuranosyl-9*H*-purin-6(1*H*)-one, *see* C-70068
2-Amino-3-chlorosuccinic acid, *see* A-70121
5-Aminocinchomeronic acid, *see* A-70195
4-Amino-3-cyano-1*H*-1,5-benzodiazepine, *see* A-70091
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3-Amino-4-cyano-1-methylpyrazole, *in* A-70187
4-Amino-3-cyano-5-methylpyrazole, *in* A-80111
5-Amino-4-cyano-1-methylpyrazole, *in* A-70192
2-Amino-5-cyanonicotinamide, *in* A-70193
3-Amino-4-cyanopyrazole, *in* A-70187
4-Amino-3-cyanopyrazole, *in* A-70189
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2-Aminocycloheptanemethanol, A-70124
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2-Amino-1,4-cyclohexanedicarboxylic acid, A-60118
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2-Amino-3-(2,4-dichlorophenyl)propanoic acid, A-60128
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7-Amino-1,6-dihydro-9*H*-imidazo[4,5-*f*]quinazolin-9-one, A-60208
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α-Amino-β,4-dihydroxybenzenebutanoic acid, *see* A-60185
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2-Amino-5-(4,5-dihydroxycyclopent-1-en-3-ylaminomethyl)pyrrolo[2,3-*d*]pyrimidine, *see* Q-70004
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2-Amino-6-hydroxy-8-iodopurine, *see* I-80031
4-Amino-6-hydroxyisophthalic acid, *see* A-70153
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5-Amino-4-hydroxyisophthalic acid, *see* A-70155
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▷ 1-Amino-4-methoxyanthraquinone, *in* A-60175
1-Amino-5-methoxyanthraquinone, *in* A-60176
9-Amino-10-methoxy-1,4-anthraquinone, *in* A-60181
3-Amino-4-methoxy-1,2-benzenedicarboxylic acid, *in* A-70151
2-Amino-4-methoxy-6-nitrotoluene, *in* A-60222
2-Amino-6-methoxyphenol, *in* A-70089
3-Amino-2-methoxyphenol, *in* A-70089
4-Amino-2-methoxyphenol, *in* A-70090
5-Amino-2-methoxyphenol, *in* A-70090
2-Amino-3-(4-methoxyphenyl)-3-methylbutanoic acid, *in* A-60198
2-Amino-4-methoxypyridine, *in* A-60253
2-Amino-6-methoxypyridine, *in* A-60252
3-Amino-2-methoxypyridine, *in* A-60249
3-Amino-4-methoxypyridine, *in* A-60254
4-Amino-2-methoxypyridine, *in* A-60250
5-Amino-2-methoxypyridine, *in* A-60251
2-Amino-4-methoxy-1,3,5-triazine, *in* A-80149
6-Amino-2-(methylamino)-4(3*H*)-pyrimidinone, *in* D-70043
2-Amino-3-methylbiphenyl, A-70164
5-Aminomethyl-3-bromoisoxazole, A-70165
2-Amino-3-methylbutanedioic acid, A-70166
1-Amino-3-methyl-2,3-butanediol, A-60216
2-Amino-2-methylbutanoic acid, A-70167
3-Amino-2-methylbutanoic acid, A-80097
3-Amino-3-methyl-2-butanol, A-60217
2-Amino-3-methyl-3-butenoic acid, A-60218
2-(Aminomethyl)-4-(carboxymethyl)-1*H*-pyrrole-3-propanoic acid, *see* I-60114
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2-(Aminomethyl)cyclohexanol, A-70169
2-(Aminomethyl)cyclooctanol, A-70170
5-(Aminomethyl)dihydro-2(3*H*)-furanone, *in* A-60196
β-Amino-α-methylene-γ-butyrolactone, *see* A-70131
2-Amino-3-methylenepentanedioic acid, A-60219
2-Amino-2-(1-methylethyl)butanedioic acid, *see* A-60212
6-Amino-2-methyl-2-hexene, *see* M-80099
2-Amino-2-methyl-3-(4-hydroxyphenyl)propanoic acid, A-60220
1-Amino-3-methylisoquinoline, A-80098
3-Amino-1-methylisoquinoline, A-80099
3-Amino-4-methylisoquinoline, A-80100
4-Amino-1-methylisoquinoline, A-80101
5-Amino-1-methylisoquinoline, A-80102
5-Amino-3-methylisoquinoline, A-80103
7-Amino-1-methylisoquinoline, A-80104
8-Amino-1-methylisoquinoline, A-80105
3-Amino-4-methylisoxazole, A-80106
4-Amino-3-methylisoxazole, A-80107
4-Amino-5-methylisoxazole, A-80108
5-Amino-4-methylisoxazole, A-80109
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2-Amino-3-methyl-1,4-naphthalenedione, *see* A-70171
2-Amino-3-methyl-1,4-naphthoquinone, A-70171
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1-(Aminomethyl)phenanthridine, *see* P-80081
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1-(2-Amino-4-methylphenyl)-2-chloroethanone, *see* A-60113
1-(2-Amino-5-methylphenyl)-2-chloroethanone, *see* A-60114
1-(2-Amino-6-methylphenyl)-2-chloroethanone, *see* A-60115
2-Amino-2-methyl-3-phenylpropanoic acid, A-60225
2-Amino-1-methyl-4(1*H*)-pteridinone, *in* A-60242
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8-Amino-9-methylpurine, *in* A-60244
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3-Amino-5-methyl-1*H*-pyrazole-4-carboxylic acid, A-80110
4-Amino-5-methyl-1*H*-pyrazole-3-carboxylic acid, A-80111
5-Amino-3-methyl-4-pyrazolecarboxylic acid, *see* A-80110
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5-Amino-2-methyl-3-pyridinol, *see* A-60193
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5-Amino-1-methyl-2(1*H*)-pyridinone, *in* A-60251
6-Amino-1-methyl-2(1*H*)-pyridinone, *in* A-60252
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2-Amino-8-methyl-9-β-D-ribofuranosyl-9*H*-purin-6(1*H*)-one, *see* M-70085
2-Amino-3-methylsuccinic acid, *see* A-70166
2-Amino-4-(*S*-methylsulfonimidoyl)butanoic acid, *see* M-70043

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5-Amino-2-methyl-2*H*-tetrazole, *in* A-70202
2-Amino-3-(methylthio)-1,4-naphthalenedione, *in* A-70163
2-Amino-5-(methylthio)pentanoic acid, A-60231
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5-Amino-2(1*H*)-pyridinone, A-60251
6-Amino-2(1*H*)-pyridinone, A-60252
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2-Amino-9-β-D-ribofuranosyl-6,8(1*H*,9*H*)-purinedione, *see* D-70238
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▷ 3-Azido-3-methyl-1-butyne, A-80203
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▷ 7-Azidonorbornadiene, *see* A-70285
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(2-Azidophenyl)phenylmethanone, *see* A-60338
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[1]-Benzopyrano[2,3-*d*]-1,2,3-triazol-9(1*H*)-one, B-60043
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3-(2-Benzothiazolyl)coumarin, *see* B-70056
N-2-Benzothiazolyl-*N*,*N*′,*N*″-triphenylguanidine, B-70057
10*H*-[1]Benzothieno[3,2-*b*]indole, B-70059
6*H*-[1]Benzothieno[2,3-*b*]indole, B-70058
[1]Benzothieno[2,3-*c*][1,5]naphthyridine, B-70060
[1]Benzothieno[2,3-*c*][1,7]naphthyridine, B-70061
[1]Benzothieno[3,2-*b*]quinoline, B-70063
[1]Benzothieno[2,3-*c*]quinoline, B-70062
[1]Benzothieno[3,2-*c*]quinoline, B-70064
3-Benzothienylglycine, *see* A-60090
1-Benzothiepin-5(4*H*)-one, B-60047
Benzothiet-2-one, B-70065
3,4-Benzothiocoumarin, *see* D-70080
Benzo[*b*]thiophen-3(2*H*)-one, B-60048
[1]Benzothiopyrano[6,5,4-*def*][1]benzothiopyran, B-60049
10*H*-[1]Benzothiopyrano[2,3-*d*]pyridazin-10-one, B-80045
1-Benzothiopyrylium(1+), B-70066
2-Benzothiopyrylium(1+), B-70067
1,2,3-Benzotriazin-4-amine, *see* A-60092
1,2,3-Benzotriazine-4-thiol, *see* B-60050
1,2,3-Benzotriazine-4(3*H*)-thione, B-60050
▷ 1*H*-Benzotriazole, B-70068
Benzo[*b*]triphenylen-10-ol, B-80050
Benzo[*b*]triphenylen-11-ol, B-80051
Benzo[*b*]triphenylen-1-ol, B-80046
Benzo[*b*]triphenylen-2-ol, B-80047
Benzo[*b*]triphenylen-3-ol, B-80048
Benzo[*b*]triphenylen-4-ol, B-80049
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tripyrazine-2,3,6,7,10,11-tetracarboxylic acid, B-60051
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1]benzothiophene, B-60052
Benzo[1,2-*b*:3,4-*b*′:6,5-*b*″]tris[1]benzothiophene, B-60053
Benzo[1,2-*d*:3,4-*d*′:5,6-*d*″]tris[1,3]dithiole, B-70069
2,3,4-Benzotrithiepin, *see* D-80176
1,2,3-Benzoxadiazole, *see* D-70057
lin-Benzoxanthine, *see* I-60009
[1,4]Benzoxaselenino[3,2-*b*]pyridine, B-60054
1,2,3-Benzoxathiazin-4(3*H*)-one, B-80052
1,3-Benzoxathiole-2-selone, B-70070
[1,4]Benzoxazino[3,2-*b*][1,4]benzoxazine, B-60055
[1,4]Benzoxazino[2,3-*b*]phenoxazine, *see* T-60378
▷ 2-Benzoxazolamine, *see* A-60093
1,5-Benzoxepine-2,4-(3*H*,5*H*)-dione, B-80053
5-Benzoylacetyl-4-methoxybenzofuran, *see* P-80169
1-[*N*-[3-(Benzoylamino)-2-hydroxy-4-phenylbutyl]alanyl]proline, B-60056
2′-*O*-Benzoylaucubin, *in* A-80186
2-Benzoylbenzoic acid, B-80054
Benzoylbenzylcarbinol, *see* H-70124
▷ 1-Benzoyl-1-bromoethane, *see* B-80243
Benzoylbutadiyne, *see* P-80114
1-Benzoyl-2-butanone, *see* P-80116
4-Benzoyl-2-butanone, *see* P-80117
1-Benzoyl-2-butene, *see* P-60127
4-Benzoylbutyraldehyde, *see* O-80094
▷ Benzoylcyclohexane, B-70071
Benzoylcyclopentane, B-80055
1-Benzoylcyclopentene, B-70072
2-Benzoyl-1,2-dihydro-1-isoquinolinecarbonitrile, B-70073
6-Benzoyl-5,7-dihydroxy-2-methyl-2-(4-methyl-3-pentenyl)chroman, B-80056
1-Benzoyl-1,1-diphenylethane, *see* T-60389
1-Benzoyl-1,2-diphenylethane, *see* T-60390
2-Benzoyl-1,1-diphenylethane, *see* T-60391
2-Benzoyl-6-geranylphloroglucinol, *in* D-80460
6-Benzoyl-1-hexene, *see* P-70080
2-Benzoylimidazole, B-70074
4(5)-Benzoylimidazole, B-60057
6-Benzoylindole, B-60058
3-Benzoylisobutyric acid, *see* B-60064
1-Benzoylisoquinoline, B-60059
3-Benzoylisoquinoline, B-60060
4-Benzoylisoquinoline, B-60061
3-Benzoylisoxazole, B-70075
4-Benzoylisoxazole, B-60062
5-Benzoylisoxazole, B-60063
5-Benzoylmethoxy-6-methoxybenzofuran, *see* P-80169
Benzoylmethylphenylmethanol, *see* H-70123
2-Benzoyl-2-methylpropane, *see* D-60443
3-Benzoyl-2-methylpropanoic acid, B-60064
2-Benzoylnaphtho[1,8-*bc*]pyran, B-70076
2-Benzoyl-6-nerylphloroglucinol, *in* D-80460
8α-Benzoyloxyacetylpringleine, *in* P-60172
1-[(Benzoyloxy)methyl]-7-oxabicyclo[4.1.0]hept-4-ene-2,3-diol 3-benzoate, *see* P-60159
1-[(Benzoyloxy)methyl]-7-oxabicyclo[4.1.0]hept-4-ene-2,3-diol diacetate, *see* S-60023
▷ 1-Benzoyl-1,3-pentadiyne, *see* P-60109
5-Benzoyl-2,4-pentadiyn-1-ol, *see* H-80235
5-Benzoyl-1-pentene, *see* P-70081
Benzoyl phenyl diselenide, B-70077
Benzoyl(phenylthio)methane, *see* P-80120
2-Benzoylpropanal, B-80057
2-Benzoylpropene, *see* M-80146
3-Benzoylpropene, *see* P-60085
2-Benzoylpropionaldehyde, *see* B-80057
3-Benzoyl-2-propyn-1-ol, *see* H-80233
3-Benzoylpyrazole, B-70078
4-Benzoylpyrazole, B-60065
5-Benzoyl-2(1*H*)-pyrimidinone, B-60066
2-Benzoylthiophenol, *see* M-70020
3-Benzoylthiophenol, *see* M-70021
4-Benzoylthiophenol, *see* M-70022
4-Benzoyl-1,2,3-triazole, B-70079
Benzoyltrichloromethane, *see* T-70219
Benzoyltriphenylmethane, *see* T-60167
Benzvalenoquinoxaline, B-70080
Benzylamine-*o*-carboxylic lactam, *see* P-70100
5-Benzylamino-1*H*-tetrazole, *in* A-70202
α-Benzylaspartic acid, *see* A-60094
2-Benzylbenzenethiol, *see* M-80024
▷ Benzyl chloroformate, *see* B-60071
1-Benzyl-3-chloropyrazole, *in* C-70155
1-Benzyl-5-chloropyrazole, *in* C-70155
Benzyldesoxybenzoin, *see* T-60390
2-*O*-Benzylglyceraldehyde, B-80058
Benzyl hydrogen 2-formylmalonate, *in* H-80204
Benzyl hydroxycarbamate, *see* B-70086
Benzyl *m*-hydroxyphenyl ether, *see* B-60073
Benzyl *o*-hydroxyphenyl ether, *see* B-60072
▷ Benzyl *p*-hydroxyphenyl ether, *see* B-60074
3-Benzylidene-4-chromanone, *see* D-60263
Benzylidenecyclobutane, B-70081
Benzylidenecycloheptane, B-60068
9-Benzylidene-1,3,5,7-cyclononatetraene, B-60069
Benzylidenecyclopentane, B-70083
1-Benzylidene-1*H*-cyclopropabenzene, B-70084
1-Benzylidene-2,3-diphenylindene, B-80059
N-Benzylidenemethylamine, B-60070
4-Benzylidene-2-phenyloxazolin-5-one, *see* P-60128
1-Benzyl-5-imino-3-methyl-1*H*,3*H*-tetrazole, *in* A-70202
3-Benzyl-5-imino-1-methyl-1*H*,3*H*-tetrazole, *in* A-70202
Benzyl isocyanate, *see* I-80055
1-Benzyl-2-mercaptobenzene, *see* M-80024
1-Benzyl-5-methylamino-1*H*-tetrazole, *in* A-70202
Benzyl orthocarbonate, *in* M-80037
2-Benzyloxyacetaldehyde, B-70085
m-Benzyloxyanisole, *in* B-60073
o-Benzyloxyanisole, *in* B-60072
p-Benzyloxyanisole, *in* B-60074
1-Benzyloxy-3-buten-2-ol, *in* B-70291
C-Benzyloxycarbohydroxamic acid, B-70086
▷ Benzyloxycarbonyl chloride, B-60071
N-Benzyloxycarbonylhydroxylamine, *see* B-70086
2-(Benzyloxy)phenol, B-60072
3-(Benzyloxy)phenol, B-60073
▷ 4-(Benzyloxy)phenol, B-60074
1-Benzyloxy-2-phenyldiazene 2-oxide, *in* H-70208
1-Benzyloxy-2-phenyldiimide 2-oxide, *in* H-70208
2-Benzyloxy-1-propanol, *in* P-70118
2-Benzylpyrrole, B-80060
3-Benzylpyrrole, B-80061
1-Benzyl-5-vinylimidazole, *in* V-70012
Benzyl vinyl sulfide, B-80062
Benzyl vinyl sulfone, *in* B-80062
Benzyl vinyl sulfoxide, *in* B-80062
Benzyne, B-70087
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Betavulgarin, *in* T-80108
Betulalbuside *A*, *in* D-80456
Betulalbuside *B*, *in* D-80456
ent-15-Beyerene-14β,19-diol, B-80064
ent-15-Beyerene-2,12-dione, B-80065
ent-15-Beyerene-3,12-dione, *in* D-80285
ent-15-Beyerene-2,3,12-trione, *in* D-80285
ent-15-Beyeren-18-oic acid, B-80066
Beyeriadiol, *in* L-60039
Bharangin, B-70088
Bharanginin, B-70089
Bhubaneswin, *in* B-70093
$\Delta^{1,1'}$-[Biacenaphthene]-2,2′-dione, *see* B-80067
1,1′-Biacenaphthylidene-2,2′-dione, B-80067

Biacenedione, *see* B-80067
9,9′-Biacridylidene, B-70090
Biadamantylidene epoxide, B-70091
Biadamantylideneethane, B-60075
Bianthrone A2a, B-60076
Bianthrone A2b, B-60077
7,7′-Bi-7-azabicyclo[2.2.1]heptane, B-80068
9,9′(10*H*,10*H*′)-Bi-9,10[1′,2′]benzenoanthracene, *see* B-80169
2,2-Bi(1,4-benzoquinone), B-80069
4,4′-Bi(1,2-benzoquinone), B-80070
2,2′-Bibenzoxazoline, *in* T-60059
Bibenzyl-2,2′-dicarboxylic acid, B-80071
7,7′-Bi(bicyclo[2.2.1]heptylidene), B-60078
9,9′-Bi(bicyclo[3.3.1]nonylidene), B-60079
5,5′-Bibicyclo[2.1.0]pentane, B-70092
1,1′-Bi(bicyclo[1.1.1]pentane)-3-carboxylic acid, B-80072
1,1′-Bibiphenylene, B-60080
2,2′-Bibiphenylene, B-60081
4,4′-Bichrysophanol, *see* S-80031
Bicolorin, *in* D-84287
Bicornin, B-80073
Bicoumol, B-70093
Bicyclo[1.1.0]butane-1-carboxylic acid, B-70094
Bicyclobutylidene, B-70095
Bicyclo[4.2.2]deca-6,8,9-triene, *see* P-60006
Bicyclo[4.3.1]deca-1(10),6,8-triene, *see* M-60029
Bicyclo[4.3.1]deca-1,3,5-trien-10-one, *see* T-70329
Bicyclo[6.2.0]dec-9-ene, B-80074
Bicyclo[4.4.0]dec-1(6)-ene-3,8-dione, *see* H-70063
Bicyclo[6.4.0]dodeca-1(8),2,4,6,10-pentaene, *see* D-70173
Bicyclo[6.2.2]dodeca-4,8,10,12-tetraene, *see* P-70010
Bicyclo[5.4.1]dodeca-7,9,11-trien-12-one, *see* T-70330
Bicyclo[8.8.2]eicosa-1(19),10(20),19-triene, B-70096
Bicyclofarnesyl epoxide, *see* D-70533
1(10),4-Bicyclogermacradien-13-oic acid, B-80075
13-Bicyclogermacrenal, B-80076
Bicyclo[14.4.1]heneicosa-1,3,5,7,9,11,13,15,17,19-decaene, B-80077
Bicyclo[3.2.0]hepta-2,6-diene, B-70097
Bicyclo[2.2.1]hepta-2,5-diene-2-carboxaldehyde, B-60083
Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, B-60084
Bicyclo[4.1.0]hepta-1(6),3-diene-2,5-dione, B-80078
Bicyclo[2.2.1]heptan-1-amine, *see* A-80060
Bicyclo[2.2.1]heptan-7-amine, *see* A-80061
Bicyclo[2.2.1]heptane-1-carboxylic acid, B-60085
Bicyclo[3.1.1]heptane-1-carboxylic acid, B-60086
▷ Bicyclo[2.2.1]heptan-2-one, B-70098
Bicyclo[4.1.0]hepta-1,3,5-triene, *see* C-70246
Bicyclo[3.1.1]hept-2-ene, B-60087
Bicyclo[4.1.0]hept-3-ene, B-80079
Bicyclo[3.2.0]hept-2-ene-6,7-dione, B-70099
Bicyclo[2.2.1]hept-5-en-2-one, B-80080
7-Bicyclo[2.2.1]hept-7-ylidenebicyclo[2.2.1]heptane, *see* B-60078
[Bi-1,4-cyclohexadien-1-yl]-3,3′,6,6′-tetrone, *see* B-80069
[Bi-1,5-cyclohexadien-1-yl]-3,3′,4,4′-tetrone, *see* B-80070
Bicyclo[2.1.1]hexan-2-amine, *see* A-70095
Bicyclo[2.1.1]hexan-2-ol, B-70100
Bicyclo[3.1.0]hexan-2-one, B-60088
[1,1′-Bicyclohexyl]-2,2′-dione, B-60089
(1,1′-Bicyclohexyl)-1,1′-diylbisbenzene, *see* D-70475
Bicyclo[12.4.1]nonadeca-1,3,5,7,9,11,13,15,17-nonaene, B-80081
Bicyclo[12.4.1]nonadec-1,3,5,7,9,11,13,15,17-nonaene, B-70101
Bicyclo[3.3.1]nona-2,6-diene, B-70102
Bicyclo[3.3.1]nonane-2,4-dione, B-70103
Bicyclo[3.3.1]nonane-2,4,7-trione, B-80082
Bicyclo[3.3.1]nonane-2,4,9-trione, B-80083
Bi(cyclononatetraenylidene), B-70104
Bicyclo[4.2.1]nona-2,4,7-trien-9-one, B-80084
Bicyclo[3.3.1]non-3-en-2-one, B-70105
Bicyclo[4.2.1]non-2-en-9-one, B-70106
Bicyclo[4.2.1]non-3-en-9-one, B-70107
Bicyclo[4.2.1]non-7-en-9-one, B-70108
Bicyclo[4.3.0]non-8-en-7-one, *see* H-70058
Bicyclo[4.1.1]octa-2,4-diene, B-60090
Bicyclo[4.2.0]octa-2,4-diene, B-80085
Bicyclo[3.3.0]octa-1,3-diene, *see* T-70075
Bicyclo[3.3.0]octa-1,4-diene, *see* T-70077
Bicyclo[3.3.0]octa-1(5),2-diene, *see* T-70076
Bicyclo[3.3.0]octa-1,5-diene, *see* T-70078
Bicyclo[3.3.0]octa-1,6-diene, *see* T-70079
Bicyclo[3.3.0]octa-1,7-diene, *see* T-70080
Bicyclo[3.3.0]octa-2,6-diene, *see* T-70081
Bicyclo[3.3.0]octa-2,7-diene, *see* T-70082
Bicyclo[2.2.2]octa-5,7-diene-2,3-dione, B-70109
▷ Bicyclo[4.2.0]octa-1,5-diene-3,4-dione, B-70110
Bicyclo[5.1.0]octa-3,5-dien-2-one, B-70111
Bicyclo[4.1.1]octane, B-60091
Bicyclo[2.2.2]octane-1-carboxylic acid, B-60092
Bicyclo[3.2.1]octane-1-carboxylic acid, B-70112
Bicyclo[4.2.0]octane-2,5-dione, B-60093
Bicyclo[3.2.1]octan-8-one, B-60094
Bicyclo[3.3.0]octa-1,3,5-triene, *see* D-70240
Bicyclo[3.3.0]octa-1,3,7-triene, *see* D-70244
Bicyclo[3.3.0]octa-1,4,6-triene, *see* D-70242
Bicyclo[3.3.0]octa-1(5),2,6-triene, *see* D-70241
Bicyclo[3.3.0]octa-1(5),2,7-triene, *see* D-70243
Bicyclo[4.1.1]oct-2-ene, B-60095
Bicyclo[4.1.1]oct-3-ene, B-60096
Bicyclo[3.3.0]oct-1(5)-ene, *see* H-70066
Bicyclo[3.3.0]oct-1-ene, *see* H-70064
Bicyclo[3.3.0]oct-2-ene, *see* H-70065
Bicyclo[2.2.2]oct-2-ene-1-carboxylic acid, B-70113
Bicyclo[2.2.2]oct-7-ene-2,5-dione, B-80086
Bicyclo[4.2.0]oct-7-ene-2,5-dione, B-60097
Bicyclo[3.2.1]oct-6-en-3-one, B-80087
Bicyclo[4.2.0]oct-2-en-7-one, B-80088
Bicyclo[3.3.0]oct-1-en-3-one, *see* T-70084
Bicyclo[3.3.0]oct-6-en-2-one, *see* T-70083
Bicyclo[18.4.1]pentacosa-1,3,5,7,9,11,13,15,17,19,21,23-dodecaene, B-80089
Bi-2,4-cyclopentadien-1-yl, B-60100
Bi-2,4-cyclopentadien-1-ylidene, *see* F-60080
Bicyclo[1.1.1]pentane-1-carboxylic acid, B-60101
Bicyclo[1.1.1]pentane-1,3-dicarboxylic acid, B-80090
[1,1′-Bicyclopropyl]-1,1′-dicarboxylic acid, B-70114
Bicyclo[6.4.1]trideca-1,3,5,7,9,11-hexaene, B-80091
Bicyclo[4.4.1]undeca-1,6-diene, B-70115
11-Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaen-11-ylidenebicyclo[4.4.1]undeca-1,3,5,7,9-pentaene, *see* B-70127
Bicyclo[5.3.1]undeca-1,4,6,8-tetraene-3,10-dione, *see* H-60086
Bicyclo[5.3.1]undeca-1,4,6,9-tetraene-3,8-dione, *see* H-60085
Bicyclo[5.3.1]undeca-3,6,8,10-tetraene-2,5-dione, *see* H-60087
4,4′-Bi[1,8-Dihydroxy-3-methylanthraquinone], *see* S-80031
2,2′-Bi(4,6-dimethyl-5*H*-1,3-dithiolo[4,5-*c*]pyrrolylidene), B-80092
Bi(1,3-diselenol-2-ylidene), B-70116
Bi(1,3-ditellurol-2-ylidene), B-70117
2,2′-Bi-1,3-dithiolane, B-60103
Bi(1,3-dithiolo[4,5-*b*][1,4]dithiin-2-ylidene), B-70118
Bi(1,3-dithiol-2-ylidene), B-70119
Bieugenol, *see* D-80023
$\Delta^{9,9'}$-Bi-9*H*-fluorene, *see* B-60104
$\Delta^{9,9'}$-Bi-9-fluorenyl, *see* B-60104
9,9′-Bifluorenylidene, B-60104
Bifurcarenone, B-80093
2,2′-Bifurylidene-5,5′-dione, B-80094
3,3′-Bi[5-hydroxy-2-methyl-1,4-naphthoquinone], B-60106
2,2′-Bi-1*H*-imidazole, B-60107
1,1′-Biindane-2,2′-dione, B-80095
2,2′-Biindane-1,1′-dione, B-80096
1,1′-Biindanylidene, B-70120
2,2′-Biindanylidene-1,1′-dione, B-80097
1,1′-Bi-1*H*-indene, B-60108
1,1′-Bi-1*H*-indene, B-80098
2,2′-Bi-1*H*-indene, B-80099
2,3′-Bi-1*H*-indene, B-80100
3,3′-Bi-1*H*-indene, B-80101
$\Delta^{1,1'}$-Biindene, B-60109
1,1′-Biindenyl, *see* B-60108
1,1′-Biindenyl, *see* B-80098
2,2′-Biindenyl, *see* B-80099
2,3′-Biindenyl, *see* B-80100
3,3′-Biindenyl, *see* B-80101
1,1′-Biindenylidene, *see* B-60109
2,2′-Biisonicotinic acid, *see* B-60126
3,3′-Biisonicotinic acid, *see* B-60134
2′,6″-Biluteolin, *see* D-70144
[1,1′-Binaphthalene]-4,4′,5,5′-tetrol, *see* T-80086
1,1′-Binaphthalene-4,4′,5,5′-tetrol, *see* T-70102
[1,1′-Binaphthalene]-3,3′,4,4′-tetrone, *see* B-80103
[2,2′-Binaphthalene]-1,1′,4,4′-tetrone, *see* B-80104
4,4′-Bi(1,2-naphthaquinone), B-80103
2,2′-Bi(1,4-naphthoquinone), B-80104
Bindschedler's green, B-60110
2,2′-Binicotinic acid, *see* B-60124
2,4′-Binicotinic acid, *see* B-60131
2,6′-Binicotinic acid, *see* B-60125
4,4′-Binicotinic acid, *see* B-60137
6,6′-Binicotinic acid, *see* B-60127
7,7′-Binorbornylidene, *see* B-60078
Biochanin *A*, *see* D-80337
▷ Biochanin B, *see* H-80190
Biopterin, B-70121
α-Biotol, B-60112
β-Biotol, B-60113
Biperezone, B-80105
[1,1′-Biphenanthrene]-2,2′,4,4′,7,7′,8,8′-octol, *see* O-80017
Biphenomycin *A*, B-60114
Biphenomycin *B*, *in* B-60114
[1,1′-Biphenyl]-2,2′-diacetic acid, B-60115
[1,1′-Biphenyl]-4,4′-diacetic acid, B-60116
[1,1′-Biphenyl]-2,2′-diamine, *see* D-60033
3,4′-Biphenyldiol, B-80106
[1,1′-Biphenyl]-4,4′-diylbis[diphenylmethyl], B-60117
2,2′-[1,1′-Biphenyl]-2,2′-diylbis-1*H*-imidazole, *see* B-70148
1-Biphenylenamine, *see* A-80062
2-Biphenylenamine, *see* A-80063
1-Biphenylenecarboxaldehyde, B-80107
2-Biphenylenecarboxaldehyde, B-80108
1-Biphenylenecarboxylic acid, B-80109
2-Biphenylenecarboxylic acid, B-80110
1,5-Biphenylenediamine, *see* D-80053
2,3-Biphenylenediamine, *see* D-80054
2,6-Biphenylenediamine, *see* D-80055
1,8-Biphenylenedicarboxaldehyde, B-60118
1,5-Biphenylenedicarboxylic acid, B-80111
1,8-Biphenylenedicarboxylic acid, B-80112
2,3-Biphenylenedicarboxylic acid, B-80113
2,6-Biphenylenedicarboxylic acid, B-80114
2,7-Biphenylenedicarboxylic acid, B-80115
1,2-Biphenylenediol, B-80116
1,5-Biphenylenediol, B-80117
1,8-Biphenylenediol, B-80118

2,3-Biphenylenediol, B-80119
2,6-Biphenylenediol, B-80120
2,7-Biphenylenediol, B-80121
1-(1-Biphenylenyl)ethanone, *see* A-80018
1-(2-Biphenylenyl)ethanone, *see* A-80019
1-Biphenylenyl methyl ketone, *see* A-80018
2-Biphenylenyl methyl ketone, *see* A-80019
[2.2](3,3′)Biphenylophane, *see* M-60031
[1,1′-Biphenyl]-2-sulfonic acid, B-80122
[1,1′-Biphenyl]-3-sulfonic acid, B-80123
[1,1′-Biphenyl]-4-sulfonic acid, B-80124
2,2′,3,4-Biphenyltetrol, B-70122
2,2′,3,4-Biphenyltetrol, B-80125
2,3,3′,4-Biphenyltetrol, B-80126
2,3,4,4′-Biphenyltetrol, B-70123
2,3,4,4′-Biphenyltetrol, B-80127
2,3′,4′,5′-Biphenyltetrol, B-80128
2,3,4-Biphenyltriol, B-70124
3,4,5-Biphenyltriol, B-80129
3,3′-Bipicolinic acid, *see* B-60133
4,4′-Bipicolinic acid, *see* B-60136
6,6′-Bipicolinic acid, *see* B-60128
3,3′-Biplumbagin, *see* B-60106
1,3(5)-Bi-1*H*-pyrazole, B-60119
▷ 2,3′-Bipyridine, B-60120
2,4′-Bipyridine, B-60121
3,3′-Bipyridine, B-60122
3,4′-Bipyridine, B-60123
[2,2′-Bipyridine]-3,3′-dicarboxylic acid, B-60124
[2,2′-Bipyridine]-3,5′-dicarboxylic acid, B-60125
[2,2′-Bipyridine]-4,4′-dicarboxylic acid, B-60126
[2,2′-Bipyridine]-5,5′-dicarboxylic acid, B-60127
[2,2′-Bipyridine]-6,6′-dicarboxylic acid, B-60128
[2,3′-Bipyridine]-2,3′-dicarboxylic acid, B-60129
[2,4′-Bipyridine]-2′,6′-dicarboxylic acid, B-60130
[2,4′-Bipyridine]-3,3′-dicarboxylic acid, B-60131
[2,4′-Bipyridine]-3′,5-dicarboxylic acid, B-60132
[3,3′-Bipyridine]-2,2′-dicarboxylic acid, B-60133
[3,3′-Bipyridine]-4,4′-dicarboxylic acid, B-60134
[3,4′-Bipyridine]-2′,6′-dicarboxylic acid, B-60135
[4,4′-Bipyridine]-2,2′-dicarboxylic acid, B-60136
[4,4′-Bipyridine]-3,3′-dicarboxylic acid, B-60137
2,4′-Bipyridine-3,5′-dicarboxylic acid, *see* B-60132
1,1′-Bipyridine-4,4′-diol, *see* D-80293
[2,2′-Bipyridine]-3,3′-diol, *see* D-80290
[2,2′-Bipyridine]-4,4′-diol, *see* D-80294
[2,2′-Bipyridine]-4,6-diol, *see* D-80296
2,2′-Bipyridine-5,5′-diol, *see* D-80297
2,2′-Bipyridine-6,6′-diol, *see* D-80299
[2,3′-Bipyridine]-3,4′-diol, *see* D-80292
[3,3′-Bipyridine]-2,2′-diol, *see* D-80287
[3,3′-Bipyridine]-4,4′-diol, *see* D-80295
3,3′-Bipyridine-5,5′-diol, *see* D-80298
3,3′-Bipyridine-6,6′-diol, *see* D-80300
[4,4′-Bipyridine]-2,2′-diol, *see* D-80288
4,4′-Bipyridine-3,3′-diol, *see* D-80291
[1,1′(2*H*,4′*H*)-Bipyridine]-2,4′-dione, *see* D-80289
[1,1′(4*H*,4′*H*)-Bipyridine]-4,4′-dione, *see* D-80293
[2,2′-Bipyridine]-4,4′(1*H*,1′*H*)-dione, *see* D-80294
[2,2′-Bipyridine]-6,6′-(1*H*,1′*H*)-dione, *see* D-80299
[3,3′-Bipyridine]-2,2′(1*H*,1′*H*)-dione, *see* D-80287
[3,3′-Bipyridine]-4,4′(1*H*,1′*H*)-dione, *see* D-80295
[3,3′-Bipyridine]-6,6′(1*H*,1′*H*)-dione, *see* D-80300
[4,4′-Bipyridine]-2,2′(1*H*,1′*H*)-dione, *see* D-80288
[2,3′-Bipyridine]-2′(1′*H*)-one, *see* H-80117
[3,3′-Bipyridine]-2(1*H*)-one, *see* H-80119
[2,2′-Bipyridin]-4-ol, *see* H-80121
[2,2′-Bipyridin]-5-ol, *see* H-80123
[2,3′-Bipyridin]-5-ol, *see* H-80124
[3,3′-Bipyridin]-5-ol, *see* H-80125
[1(2*H*),2′-Bipyridin]-2-one, *see* P-80219
[1(2*H*),4′-Bipyridin]-2-one, *see* P-80222
[1(4*H*),2′-Bipyridin]-4-one, *see* P-80220
[1(4*H*),3′-Bipyridin]-4-one, *see* P-80221
[1(4*H*),4′-Bipyridin]-4-one, *see* P-80223
[2,2′-Bipyridin]-6(1*H*)one, *see* H-80126
[2,3′-Bipyridin]-6(1*H*)-one, *see* H-80127
[2,4′-Bipyridin]-2′(1*H*)-one, *see* H-80118
[2,4′-Bipyridin]-6(1*H*)-one, *see* H-80128
[3,3′-Bipyridin]-4(1*H*)-one, *see* H-80122
[3,3′-Bipyridin]-6(1*H*)-one, *see* H-80129
[3,4′-Bipyridin]-6(1*H*)-one, *see* H-80130
[4,4′-Bipyridin]-2(1*H*)-one, *see* H-80120
1,1′-Bi-4-pyridone, *see* D-80293
2,2′-Bi-4-pyridone, *see* D-80294
3,3′-Bi-2-pyridone, *see* D-80287
3,3′-Bi-4-pyridone, *see* D-80295
4,4′-Bi-2-pyridone, *see* D-80288
5,5′-Bi-2-pyridone, *see* D-80300
6,6′-Bi-2-pyridone, *see* D-80299
2,4′-Bipyridyl, *see* B-60121
3,3′-Bipyridyl, *see* B-60122
3,4′-Bipyridyl, *see* B-60123
2,2′-Bipyridyl-3,3′-dicarboxylic acid, *see* B-60124
2,2′-Bipyridyl-3,5′-dicarboxylic acid, *see* B-60125
2,2′-Bipyridyl-4,4′-dicarboxylic acid, *see* B-60126
2,2′-Bipyridyl-5,5′-dicarboxylic acid, *see* B-60127
2,2′-Bipyridyl-6,6′-dicarboxylic acid, *see* B-60128
2,3′-Bipyridyl-2′,3-dicarboxylic acid, *see* B-60129
2,4′-Bipyridyl-2′,6′-dicarboxylic acid, *see* B-60130
2,4′-Bipyridyl-3,3′-dicarboxylic acid, *see* B-60131
3,3′-Bipyridyl-2,2′-dicarboxylic acid, *see* B-60133
3,3′-Bipyridyl-4,4′-dicarboxylic acid, *see* B-60134
3,4′-Bipyridyl-2′,6′-dicarboxylic acid, *see* B-60135
4,4′-Bipyridyl-2,2′-dicarboxylic acid, *see* B-60136
4,4′-Bipyridyl-3,3′-dicarboxylic acid, *see* B-60137
2,2′-Bi-1*H*-pyrrole-5-carboxaldehyde, B-80130
[1,1′-Bipyrrolidine]-2,2′-dione, B-70125
Biquadricyclenylidene, B-80131
4,4′-Biquinaldine, *see* D-60413
1,10-Bisaboladiene-3,6-diol, B-80132
3,10-Bisaboladiene-7,14-diol, B-80133
Bisabolangelone, B-60138
β-Bisabolene, B-80134
10-Bisabolene-7,15-diol, B-80135
2-Bisabolene-1,12-diol, B-70126
11-Bisabolene-7,10,15-triol, B-80136
5,6-Bis(acetyloxy)-10-chloro-12-hydroxy-9-oxoprosta-7,10,14,17-tetraen-1-oic acid methyl ester, *see* P-70143
▷ 6,16-Bis(acetyloxy)-3,7-dioxo-29-nordammara-1,17(20),24-trien-21-oic acid, *see* H-80011
1,3-Bis(allylthio)cyclobutane, *in* C-60184
1,2-Bis(2-aminoethoxy)ethane, B-60139
3,3-Bis(aminomethyl)oxetane, B-60140
1,1:2,2-Bis([10]annulene-1,6-diyl)ethylene, B-70127
2,3-Bis(9-anthryl)cyclopropenone, B-70128
Bis(1-azabicyclo[2.2.2]octane)bromine(1+), *see* B-60173
▷ Bis(benzenesulfonyl)peroxide, *see* B-70018
6*H*,24*H*,26*H*,38*H*,56*H*,58*H*-16,65:48,66-Bis([1,3]benzenomethanothiomethano[1,3]benzeno)-32,64-etheno-1,5:9,13:14,18:19,23:27,31:33,37:41,45:46,50:51,55:59,63-decemetheno-8*H*,40*H*[1,7]dithiacyclotetratriacontino[9,8-*h*][1,77]dithiocyclotetratriacontin, B-70129
1,2-Bis(4′-benzo-15-crown-5)diazene, B-60141
1,2-Bis(4′-benzo-15-crown-5)ethene, B-60142
Bisbenzo[3,4]cyclobuta[1,2-*c*;1′,2′-*g*]phenanthrene, B-60143
Bis(benzothiazolo)[3,2-*b*:3′,2″-*e*][1,2,4,5]tetrazine, *see* T-60171
1,1′-Bisbiphenylenyl, *see* B-60080
2,2′-Bisbiphenylenyl, *see* B-60081
1,4-Bis[5-(4-biphenylyl)-2-oxazolyl]benzene, *see* P-60091
N,*N*-Bis([2,2′-bipyridin]-6-ylmethyl)[2,2′-bipyridine]-6-methanamine, *see* T-70320
N,*N*′-Bis[3-(3-bromo-4-hydroxyphenyl)-2-oximidopropionyl]cystamine, B-70130
2,3-Bis(bromomethyl)-1,4-dibromobutane, B-60144
1,2-Bis(bromomethyl)-3-fluorobenzene, B-70131
1,2-Bis(bromomethyl)-4-fluorobenzene, B-70132
1,3-Bis(bromomethyl)-2-fluorobenzene, B-70133
1,3-Bis(bromomethyl)-5-nitrobenzene, B-60145
▷ 2,6-Bis(bromomethyl)pyridine, B-60146
3,5-Bis(bromomethyl)pyridine, B-60147
2,3-Bis(bromomethyl)thiopene, B-80137
2,5-Bis(bromomethyl)thiophene, B-80138
3,4-Bis(bromomethyl)thiophene, B-80139
Bis(2-bromophenyl)ethyne, B-80140
Bis(4-bromophenyl)ethyne, B-80141
Bis(2-carboxyethyl)ether, *see* O-80098
4,4-Bis(2-carboxyethyl)heptanedioic acid, *see* M-70036
2,2′-Bis(carboxymethyl)biphenyl, *see* B-60115
4,4′-Bis(carboxymethyl)biphenyl, *see* B-60116
▷ 3,12-Bis(carboxymethyl)-6,9-dioxa-3,12-diazatetradecanedioic acid, B-70134
N,*N*′-Bis(carboxymethyl)urea, *see* C-80020
1,2-Bis(2-carboxyphenyl)ethane, *see* B-80071
Bis(chlorocarbonyl) disulfide, B-80142
2,3-Bis(chloromethyl)-1,4-dichlorobutane, B-60148
▷ 3,3-Bis(chloromethyl)oxetane, B-60149
2,4-Bis(chloromethyl)pyridine, B-80143
Bis(2-cyanoethyl)ether, *in* O-80098
2,2′-Bis(cyanomethyl)biphenyl, *in* B-60115
4,4′-Bis(cyanomethyl)biphenyl, *in* B-60116
1,2-Bis(cyclohexylidene)ethene, B-80144
Biscyclolobin, B-80145
1,1′-Bis(cyclopentadienylidene), *see* F-60080
Bisdemethoxycurcumin, *in* C-80165
2,3-Bis(dibromomethyl)pyrazine, B-60150
2,3-Bis(dibromomethyl)pyridine, B-60151
3,4-Bis(dibromomethyl)pyridine, B-60152
4,5-Bis(dibromomethyl)pyrimidine, B-60153
Bis(2,4-dichlorophenyl)ether, B-70135
Bis(2,6-dichlorophenyl) ether, B-70136
Bis(3,4-dichlorophenyl) ether, B-70137
Bis(1,1-dicyclopropylmethyl)diazene, B-60154
2,6-Bis(3,4-Dihydro-2*H*-pyrrol-5-yl)pyridine, B-80146
Bisdihydrotrifarin, *in* T-70236
1,5-Bis(3,4-dihydroxyphenyl)-1,2-dihydroxy-4-pentyne, *see* B-60155
1,2-Bis(3,4-dihydroxyphenyl)ethane, *see* T-60101
1,5-Bis(3,4-dihydroxyphenyl)-4-pentyne-1,2-diol, B-60155
3,6-Bis(3,4-dimethoxyphenyl)tetrahydro-1*H*,3*H*-furo[3,4-*c*]furan-1,4-diol, B-60156
▷ 4,4′-Bisdimethylaminobenzophenone imide, *see* A-70268
2,2′-Bis(dimethylamino)biphenyl, *in* D-60033
▷ Bis(dimethylamino)diazene, *see* T-80153

1,8-Bis(dimethylamino)naphthalene, *in* D-70042
1,3-Bis(dimethylamino)pentalene, B-80147
▷ Bis(4-dimethylaminophenyl)methylenimine, *see* A-70268
1,1-Bis(1,1-dimethylethyl)cyclopropane, *see* D-60112
3,7-Bis(1,1-dimethylethyl)-9,10-dimethyl-2,6-anthracenedione, *see* D-60113
Bis[1-(1,1-dimethylethyl)-2,2-dimethylpropyl]diazene, *see* T-60024
2,6-Bis(1,1-dimethylethyl)-1-nitronaphthalene, *see* D-80109
3,7-Bis(1,1-dimethylethyl)-1-nitronaphthalene, *see* D-80110
5-[3,5-Bis(1,1-dimethylethyl)-4-oxo-2,5-cyclohexadien-1-ylidene]-3,6-cycloheptadiene-1,2-dione, *see* D-70105
2,6-Bis(1,1-dimethylethyl)piperidine, *see* D-80111
3,4-Bis(1,1-dimethylethyl)pyrazole, *see* D-70106
3,5-Bis(1,1-dimethylethyl)pyrazole, *see* D-70107
3,6-Bis(1,1-dimethylethyl)pyrrolo[3,2-*b*]pyrrole, *see* D-70108
3,4-Bis(1,1-dimethylethyl)-2,2,5,5-tetramethylhexane, *see* D-70109
2,4-Bis(1,1-dimethylethyl)thiophene, *see* D-80112
S,S-Bis(4,6-dimethyl-2-pyrimidinyl)dithiocarbonate, B-70138
Bis(2,5-dimethylpyrrolo[3,4-*d*]tetrathiafulvene), *see* B-80092
Bisdiphenylazimethylene, *see* D-80512
1,3-Bis(1,2-diphenylethenyl)benzene, B-70139
1,4-Bis(1,2-diphenylethenyl)benzene, B-70140
Bis(diphenylmethyl)amine, *see* T-70150
Bis(diphenylmethyl) diselenide, B-70141
3,6-Bis(diphenylmethylene)-1,4-cyclohexadiene, B-60157
1,3-Bis(1,2-diphenylvinyl)benzene, *see* B-70139
1,4-Bis(1,2-diphenylvinyl)benzene, *see* B-70140
Bis(dithiobenzoic) thioanhydride, *see* B-80013
1,11-Bisepicaniojane, *in* C-70013
7,8,9,10-Bisepoxydispiro[2.0.2.4]decane, *see* D-60500
1,2;3,4-Bisepoxy-11(13)-eudesmen-12,8-olide, B-70142
Bis(ethylenedithio)benzene, *see* T-70039
Bis(ethylenedithio)tetrathiafulvalene, *see* D-60238
Bis(ethyleneoxythio)benzene, *see* T-70040
▷ Bis(2-ethylhexyl)adipate, B-80148
Bis(2-ethylhexyl) decanedioate, B-80149
Bis(2-ethylhexyl) sebacate, *see* B-80149
1,2-Bis(ethylidene)cyclohexane, *see* D-70154
4,6-Bis(ethylthio)-2,5-dihydropyrimidine, *in* D-70257
1,4-Bis(ethylthio)-3,6-diphenyl-2,5-diazapentalene, *see* B-60158
1,4-Bis(ethylthio)-3,6-diphenylpyrrolo[3,4-*c*]pyrrole, B-60158
1,11-Bis(3-furanyl)-4,8-dimethyl-3,6,8-undecatrien-2-ol, B-70143
N^1,N^8-Bis(glutathionyl)spermidine, *see* T-70331
Bis(homoadamantane), *see* H-70031
Bishomoanthraquinone, *see* T-60264
1,4-Bishomohexaprismane, *see* H-70013
Bis-homotris, *see* A-80085
1,2-Bis(hydrazino)ethane, *see* D-60192
2,6-Bis(hydroxyacetyl)pyridine, B-70144
Bis(3-hydroxycyclobutyl)disulfide, *in* M-60019
S,S'-Bis(2-hydroxyethyl)-1,2-ethanedithiol, B-70145
1,2-Bis(2-hydroxyethylthio)ethane, *see* B-70145
1,12-Bis(3-hydroxy-5-methoxy-4-methylphenyl)dodecane, *see* M-80002
1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, *see* C-80165
1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol, B-80150
2,3-Bis(hydroxymethyl)-1,4-butanediol, B-60159
7,11-Bis(hydroxymethyl)-3,15-dimethyl-2,6,10,14-hexadecatetraen-1-ol, B-80151
2,5-Bis(hydroxymethyl)furan, B-60160
3,4-Bis(hydroxymethyl)furan, B-60161
1,7-Bis(hydroxymethyl)-7-methylbicyclo[2.2.1]heptan-2-ol, B-70146
▷ Bis(hydroxymethyl)nitromethane, *see* N-60038
3,3-Bis(hydroxymethyl)oxetane, *see* O-60056
3,6-Bis(hydroxymethyl)phenanthrene, *see* P-60069
4,5-Bis(hydroxymethyl)phenanthrene, *see* P-60070
2,5-Bis(4-hydroxyphenyl)-3,4-dimethyltetrahydrofuran, *see* T-60061
1,2-Bis(2-hydroxyphenyl)ethylene, *see* D-80378
1,2-Bis(3-hydroxyphenyl)ethylene, *see* D-80381
1,2-Bis(4-hydroxyphenyl)ethylene, *see* D-80385
1,7-Bis(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, *in* C-80165
1,5-Bis(4-hydroxyphenyl)-1,4-pentadiene, B-60162
1,2-Bis(4-hydroxyphenyl)-1,2-propanediol, B-70147
1,3-Bis(4-hydroxyphenyl)-2-propen-1-one, B-80152
Bis(3-hydroxypropyl) ether, *see* O-60097
▷ Bis(1-hydroxy-2(1*H*)-pyridinethionato-*O,S*)zinc, *in* P-60224
2,2'-Bis(2-imidazolyl)biphenyl, B-70148
Bis(2-imidazolyl)ketone, *see* D-70354
4,8-Bis-*epi*-inuviscolide, *in* I-70023
1,2-Bis(2-iodoethoxy)ethane, B-60163
Bis(2-iodoethyl) ether, *see* O-60096
2,5-Bis(iodomethyl)thiophene, B-80153
▷ 1,4-Bis(1-isocyanato-1-methylethyl)benzene, B-70149
S,S'-Bis(2-mercaptoethyl)-1,2-ethanedithiol, B-70150
1,1-Bis(mercaptomethyl)cyclobutane, *see* C-70213
1,2-Bis(mercaptomethyl)cyclobutane, *see* C-70214
1,1-Bis(mercaptomethyl)cyclohexane, *see* C-70223
1,2-Bis(mercaptomethyl)cyclohexane, *see* C-70224
1,1-Bis(mercaptomethyl)cyclopentane, *see* C-70243
1,1-Bis(mercaptomethyl)cyclopropane, *see* C-70249
2,2-Bis(mercaptomethyl)-1,3-propanedithiol, B-60164
2,5-Bis(mercaptomethyl)thiophene, *see* T-70184
2,6-Bis(mercaptomethyl)toluene, *see* M-70050
1,6:7,12-Bismethano[14]annulene, B-60165
2,6-Bis(methoxyacetyl)pyridine, *in* B-70144
1,3-Bis[(2-methoxyethoxy)methoxy]-1,3-diphenyl-2-propanone, B-80154
2,3-Bis(2-methoxy-4-nitro-5-sulfophenyl)-5-[(phenylamino)carbonyl]-2*H*-tetrazolium hydroxide inner salt, B-70151
2,2'-Bis(methylamino)biphenyl, *in* D-60033
1,8-Bis(methylamino)naphthalene, *in* D-70042
2,4-Bis(3-methyl-2-butenyl)phenol, B-80155
2,3-Bis(methylene)bicyclo[2.2.1]heptane, *see* D-70405
2,6-Bis(methylene)bicyclo[3.3.1]nonane, *see* D-80448
6,7-Bis(methylene)bicyclo[3.2.2]nonane, *see* D-70406
7,8-Bis(methylene)bicyclo[2.2.2]octa-2,5-diene, *see* D-70407
2,3-Bis(methylene)bicyclo[2.2.2]octane, *see* D-70408
Bis(methylene)bicyclo[1.1.1]pentanone, *see* D-60422
Bis(methylene)butanedinitrile, *in* D-70409
Bis(methylene)butanedioic acid, *see* D-70409
1,2-Bis(methylene)cyclohexane, B-60166
1,3-Bis(methylene)cyclohexane, B-60167
1,4-Bis(methylene)cyclohexane, B-60168
1,2-Bis(methylene)cyclopentane, B-60169
1,3-Bis(methylene)cyclopentane, B-60170
2,3-Bis(3,4-methylenedioxybenzyl)butane, *see* A-70270
3,4;3',4'-Bis(methylenedioxy)bibenzyl, *in* T-60101
4,5;4',5'-Bismethylenedioxypolemannone, *in* P-60166
9,10-Bis(methylene)tricyclo[5.3.0.0^{2,8}]deca-3,5-diene, B-70152
Bis(1-methylethyl)cyanamide, *see* D-60392
1,1'-[1,2-Bis(1-methylethylidene)-1,2-ethanediyl]bisbenzene, *see* D-60419
3,3-Bis(methylnitraminomethyl)oxetane, *in* B-60140
3,6-Bis(1-methylpropyl)-2,5-piperazinedione, B-70153
3,6-Bis(2-methylpropyl)-2,5-piperazinedione, B-60171
Bis(methylsulfonyl) peroxide, B-70154
2,3-Bis(methylsulfonyl)pyridine, *in* P-60218
2,4-Bis(methylsulfonyl)pyridine, *in* M-80029
2,5-Bis(methylsulfonyl)pyridine, *in* P-60220
3,5-Bis(methylsulfonyl)pyridine, *in* P-60222
2,3-Bis(methylthio)-1,4-benzenediamine, *in* D-60030
2,3-Bis(methylthio)-1,4-benzenediamine, *in* D-70036
[Bis(methylthio)methylene]propanedinitrile, *in* D-60395
3,3-Bis(methylthio)propenal, B-80156
3,6-Bis(methylthio)pyridazine, *in* M-80028
2,3-Bis(methylthio)pyridine, *in* P-60218
2,4-Bis(methylthio)pyridine, *in* M-80029
2,4-Bis(methylthio)pyridine, *in* P-60219
2,5-Bis(methylthio)pyridine, *in* P-60220
3,5-Bis(methylthio)pyridine, *in* P-60222
2,5-Bis(methylthio)-1,3,4-thiadiazole, *in* M-70031
2,5-Bis(methylthio)-*p*-xylene, *in* D-60406
3,3-Bis(nitratomethyl)oxetane, *in* O-60056
Bis(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)diazene, *see* B-60141
Bisparthenolidine, B-80157
Bis(pentafluorophenyl)methane, B-80158
1,4-Bis(pentamethylene)-1,2,3-butatriene, *see* B-80144
1',2'-Bis(2,5,8,11,14-pentaoxabicyclo[13.4.0]nonadeca-1(15),16,18-trien-17-yl)ethene, *see* B-60142
Bis-*peri*-phenylenenaphthalene, *see* I-80010
1,1'-Bis(1,3-phenylene)naphthalene, *see* D-60454
2,2'-Bis(1,3-phenylene)naphthalene, *see* D-60455
Bis(phenylmethyl)diselenide, *see* D-60082
2,3-Bis(phenylseleno)-2-butenedioic acid, B-80159
1,2-Bis(phenylsulfinyl)cyclobutene, *in* B-70156
1,2-Bis(phenylsulfonyl)cyclobutene, *in* B-70156
▷ Bis(phenylsulfonyl)peroxide, *see* B-70018
S,S'-Bis(1-phenyl-1*H*-tetrazol-5-yl) dithiocarbonate, B-70155
1,2-Bis(phenylthio)cyclobutene, B-70156
3,3-Bis(phenylthio)propanoic acid, B-70157
3,3-Bis(phenylthio)-1-propanol, B-70158
1,4-Bis(2-propynyloxy)-2-butyne, *see* D-80499
1,4-Bis(2-pyridylamino)phthalazine, B-60172
2,6-Bis(2-pyrrolidinyl)pyridine, B-80160
Bis(quinuclidine)bromine(1+), B-60173
Bissetone, B-60174
Bis(β-styryl)selenide, *see* D-60503
N,N'-Bis(3-sulfonatopropyl)-2,2'-bipyridinium, B-70159

N,N'-Bis(3-sulfonatopropyl)-4,4'-bipyridinium, B-70160
1,1'-Bis(3-sulfopropyl)-2,2'-bipyridinium dihydroxide bis(inner salt), *see* B-70159
1,1'-Bis(3-sulfopropyl)-4,4'-bipyridinium dihydroxide bis(inner salt), *see* B-70160
Bistheonellide *A*, *see* M-60138
Bistheonellide *B*, *in* M-60138
Bis[1,2,5-thiadiazolo][3,4-*b*:3',4'-*e*]pyrazine, B-70161
1,1-Bis(thiomethyl)cyclobutane, *see* C-70213
1,2-Bis(thiomethyl)cyclobutane, *see* C-70214
1,1-Bis(thiomethyl)cyclohexane, *see* C-70223
1,2-Bis(thiomethyl)cyclohexane, *see* C-70224
1,1-Bis(thiomethyl)cyclopropane, *see* C-70249
2,5-Bis(thiomethyl)thiophene, *see* T-70184
2,6-Bis(thiomethyl)toluene, *see* M-70050
Bis(2,4,6-tri-*tert*-butylphenyl)ditellane, *see* B-70162
Bis(2,4,6-tri-*tert*-butylphenyl)ditelluride, B-70162
Bis(trichloromethyl) carbonate, B-70163
[Bis(trifluoroacetoxy)iodo]pentafluorobenzene, B-80161
1,4-Bis(trifluoroethenyl)benzene, *see* B-80165
1,2-Bis(trifluoromethyl)benzene, B-60175
1,3-Bis(trifluoromethyl)benzene, B-60176
1,4-Bis(trifluoromethyl)benzene, B-60177
3,3-Bis(trifluoromethyl)-3*H*-diazirine, B-60178
Bis-α-trifluoromethyldifluoroethane-β-sultone, *see* D-60181
4,5-Bis(trifluoromethyl)-1,3,2-dithiazol-2-yl, B-70164
3,4-Bis(trifluoromethyl)-1,2-dithiete, B-60179
N,N-Bis(trifluoromethyl)hydroxylamine, B-60180
2,3-Bis(trifluoromethyl)pyridine, B-60181
2,4-Bis(trifluoromethyl)pyridine, B-60182
2,5-Bis(trifluoromethyl)pyridine, B-60183
2,6-Bis(trifluoromethyl)pyridine, B-60184
3,4-Bis(trifluoromethyl)pyridine, B-60185
3,5-Bis(trifluoromethyl)pyridine, B-60186
Bis(trifluoromethyl)sulfene, B-80162
Bis[(trifluoromethyl)thio]acetylene, B-80163
1,2-Bis[(trifluoromethyl)thio]ethene, B-80164
Bis(trifluoromethyl)thioketene, B-60187
2,4-Bis[2,2,2-Trifluoro-1-(trifluoromethyl)ethylidene]-1,3-dithietane, B-60188
1,4-Bis(trifluorovinyl)benzene, B-80165
1,2-Bis(3,4,5-trihydroxyphenyl)ethane, *see* H-60062
Bis[2,4,6-tris(1,1-dimethylethyl)phenyl]ditelluride, *see* B-70162
Bis(vinylenedithio)tetrathiafulvalene, *see* B-70118
1,1'-Bitetralinylidene, B-70165
2,2'-Bithiazole, B-70166
2,4'-Bithiazole, B-70167
2,5'-Bithiazole, B-70168
4,4'-Bithiazole, B-70169
4,5'-Bithiazole, B-70170
5,5'-Bithiazole, B-70171
4-[2,2'-Bithiophen]-5-yl-3-butyne-1,2-diol, B-80166
4-[2,2'-Bithiophen-5-yl]-3-butyn-1-ol, B-80167
α,α'-Bi-*o*-toluic acid, *see* B-80071
4,4'-Bi-1*H*-1,2,3-triazole, B-80168
4,4'-Bi-4*H*-1,2,4-triazole, B-60189
3,3'-Bi(4',5,7-trihydroxyflavanone), *see* I-70064
9,9'-Bitriptycyl, B-80169
9,9'-Bitryptycene, *see* B-80169
Biuret, B-60190
Blastidic acid, B-80170
Blastmycetin *D*, B-60191
▷ Blastostimulina, *in* T-80343
Blumealactone *A*, *in* B-70172
Blumealactone *B*, *in* B-70172
Blumealactone *C*, B-70172
BMY 28100, *see* A-70221
Boesenboxide, B-70173
Bomag, *in* O-70102
Bonafousioside, B-80171
Bonducellin, B-60192
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2,5-Bornanediol, *see* T-70280
2,3,10-Bornanetriol, *see* H-70173
2,8,10-Bornanetriol, *see* B-70146
Boronolide, B-60193
Botrylactone, B-70174
▷ Botryodiplodin, B-60194
▷ Bovolide, *see* D-70430
Bowdichione, B-70175
Boxazomycin *A*, B-70176
Boxazomycin *B*, *in* B-70176
Boxazomycin *C*, *in* B-70176
Brachycarpone, B-60195
Brachynereolide, B-60196
Brassicadiol, B-70177
Brassinolide, B-70178
Brasudol, B-60197
Brayleanin, *in* C-60026
α-Brazanquinone, *see* B-60033
β-Brazanquinone, *see* B-60034
Bretonin A, *in* D-80526
Brevifloralactone, B-70179
Brevifloralactone acetate, *in* B-70179
Brevifolin, *in* T-70248
Brianthein V, B-80172
Brivudine, *see* B-80266
2-Bromo-5-formylfuran, *see* B-60259
3-Bromo-2-formylfuran, *see* B-60257
4-Bromo-2-formylfuran, *see* B-60258
10-Bromo-9(10*H*)-anthracenone, *see* B-80173
10-Bromoanthrone, B-80173
3-Bromoaspartic acid, *see* A-70098
1-Bromobenz[*a*]anthracene, B-80174
2-Bromobenz[*a*]anthracene, B-80175
3-Bromobenz[*a*]anthracene, B-80176
4-Bromobenz[*a*]anthracene, B-80177
▷ 7-Bromobenz[*a*]anthracene, B-80178
2-Bromo-1,3,5-benzenetriol, B-60199
3-Bromo-1,2,4-benzenetriol, B-70180
4-Bromo-1,2,3-benzenetriol, B-60200
5-Bromo-1,2,3-benzenetriol, B-60201
5-Bromo-1,2,4-benzenetriol, B-70181
6-Bromo-1,2,4-benzenetriol, B-70182
p-Bromobenzhydrol, *see* B-60236
1-Bromo-2,3-benzobicyclo[2.2.1]hepta-2,5-diene, *see* B-60231
2-Bromobenzocyclopropene, B-60202
3-Bromobenzocyclopropene, B-60203
1-Bromobenzonorbornadiene, *see* B-60231
2-Bromobenzonorbornadiene, *see* B-60232
7-Bromobenzonorbornadiene, *see* B-60233
9-Bromobenzonorbornadiene, *see* B-60233
3-Bromo-4*H*-1-benzopyran-4-one, B-70183
2-Bromobenzo[*b*]thiophene, B-60204
3-Bromobenzo[*b*]thiophene, B-60205
4-Bromobenzo[*b*]thiophene, B-60206
5-Bromobenzo[*b*]thiophene, B-60207
6-Bromobenzo[*b*]thiophene, B-60208
7-Bromobenzo[*b*]thiophene, B-60209
2-Bromobicyclo[2.2.1]heptane-1-carboxylic acid, B-60210
2-Bromobicyclo[4.1.0]hepta-1,3,5-triene, *see* B-60202
3-Bromobicyclo[4.1.0]hepta-1,3,5-triene, *see* B-60203
2-Bromobicyclo[2.2.1]hept-2-ene, B-80179
1-Bromobicyclo[2.2.2]octane, B-70184
1-Bromobicyclo[2.2.2]octane, B-80180
3-Bromo[1,1'-biphenyl]-4-carboxylic acid, B-60211
1-Bromobiphenylene, B-80181
2-Bromobiphenylene, B-80182
2-Bromo-3,3'-bipyridine, B-70185
4-Bromo-2,2'-bipyridine, B-70186
5-Bromo-2,3'-bipyridine, B-70187
5-Bromo-2,4'-bipyridine, B-70188
5-Bromo-3,3'-bipyridine, B-70189
5-Bromo-3,4'-bipyridine, B-70190
6-Bromo-2,2'-bipyridine, B-70191
6-Bromo-2,3'-bipyridine, B-70192
6-Bromo-2,4'-bipyridine, B-70193
3-Bromo-2-(3-bromo-4,5-dihydroxybenzyl)-4,5-dihydroxybenzyl alcohol, *see* B-70194
3-Bromo-4-[(3-bromo-4,5-dihydroxyphenyl)methyl]-5-(hydroxymethyl)-1,2-benzenediol, B-70194
▷ 1-Bromo-2-(bromomethyl)naphthalene, B-60212
1-Bromo-4-(bromomethyl)naphthalene, B-60213
1-Bromo-5-(bromomethyl)naphthalene, B-60214
1-Bromo-7-(bromomethyl)naphthalene, B-60215
1-Bromo-8-(bromomethyl)naphthalene, B-60216
2-Bromo-3-(bromomethyl)naphthalene, B-60217
2-Bromo-6-(bromomethyl)naphthalene, B-60218
3-Bromo-1-(bromomethyl)naphthalene, B-60219
6-Bromo-1-(bromomethyl)naphthalene, B-60220
7-Bromo-1-(bromomethyl)naphthalene, B-60221
7-Bromo-4-(1-bromopropyl)-2-(2-penten-4-ynyl)-3,9-dioxabicyclo[4.2.1]nonane, *see* I-70067
1-Bromo-1,2-butadiene, B-70196
4-Bromobutanal, B-70197
Bromo-*tert*-butylacetylene, *see* B-70207
2-(4-Bromobutyl)-1,3-dioxole, *in* B-70263
4-Bromo-1-butyne, B-70198
3-Bromo-1-butynylbenzene, *see* B-60314
3-Bromobutyrine, *see* A-60097
4-Bromobutyrine, *see* A-60098
Bromocarbonimidic difluoride, B-80183
2-Bromo-4-carboxybenzenethiol, *see* B-70228
3-Bromo-4-carboxybenzenethiol, *see* B-70226
4-Bromo-3-carboxybenzenethiol, *see* B-70227
10-Bromo-2,7-chamigradiene, B-80184
10-Bromo-α-chamigrene, *see* B-80184
5-Bromo-7-chlorocavernicolin, B-70199
2-Bromo-4-chloro-1-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane, B-80185
1-Bromo-6-chlorohexane, B-70200
10*R*-Bromo-4-chloro-9*S*-hydroxy-3,7(14)-chamigradiene, *see* E-70002
3-(3-Bromo-4-chloro-4-methylcyclohexyl)-2-methylfuran, *see* F-60090
5-(3-Bromo-4-chloro-4-methylcyclohexyl)-5-methyl-2(5*H*)-furanone, B-60222
3-Bromo-5-chloropyridine, B-60223
4-Bromo-3-chloropyridine, B-60224
▷ 1-Bromo-2-chloro-1,1,2-trifluoroethane, B-80186
3-Bromochromone, *see* B-70183
1-Bromochrysene, B-80187
2-Bromochrysene, B-80188
3-Bromochrysene, B-80189
4-Bromochrysene, B-80190
5-Bromochrysene, B-80191
6-Bromochrysene, B-80192
3-Bromo-4-cyanobiphenyl, *in* B-60211
2-Bromo-2-cyanopropane, *in* B-80229
2-Bromo-1,3-cyclohexanedione, B-70201
5-Bromodecahydro-α,α,4*a*-trimethyl-8-methylene-2-naphthalenemethanol, *see* B-60197
5-Bromo-5-decene, B-60225
4-Bromo-2,3-dichloroanisole, *in* B-60229
2-Bromo-4,5-dichloro-1-(2-chlorovinyl)-1,5-dimethylcyclohexane, *see* M-80035
2-Bromo-1,2-dichloro-1,1-difluoroethane, B-80193
1-Bromo-2,3-dichloro-4-methoxybenzene, *in* B-60229
2-Bromo-3,5-dichlorophenol, B-60226
2-Bromo-4,5-dichlorophenol, B-60227
3-Bromo-2,4-dichlorophenol, B-60228
4-Bromo-2,3-dichlorophenol, B-60229
4-Bromo-3,5-dichlorophenol, B-60230

4-Bromo-4,4-difluoro-2-butynoic acid, B-70202
1-Bromo-1,2-difluoroethene, *see* B-80194
1-Bromo-1,2-difluoroethylene, B-80194
1-Bromo-3,3-difluoro-2-iodocyclopropene, B-80195
1-Bromo-1,1-difluoro-2-iodoethane, B-80196
N-Bromo-1,1-difluoromethanimine, *see* B-80183
(Bromodifluoromethyl)phenylacetylene, *see* B-70203
3-Bromo-3,3-difluoro-1-phenylpropyne, B-70203
(3-Bromo-3,3-difluoro-1-propynyl)benzene, *see* B-70203
1-Bromo-1,4-dihydro-1,4-methanonaphthalene, B-60231
2-Bromo-1,4-dihydro-1,4-methanonaphthalene, B-60232
9-Bromo-1,4-dihydro-1,4-methanonaphthalene, B-60233
1-Bromo-3,4-dihydro-2-naphthalenecarboxaldehyde, B-80197
2-Bromo-3,4-dihydro-1-naphthalenecarboxaldehyde, B-80198
7-Bromo-3,4-dihydro-1(2*H*)-naphthalenone, B-60234
2-Bromodihydroresorcinol, *see* B-70201
3-Bromo-2,3-dihydrothiophene, B-70204
5-Bromo-3,4-dihydro-4-thioxo-2(1*H*)-pyrimidinone, B-70205
(4-Bromo-2,5-dihydroxyphenyl)(2,6-dimethyl-6-hydroxy-2-heptenyl)ketone, *see* B-70206
1-(4-Bromo-2,5-dihydroxyphenyl)-7-hydroxy-3,7-dimethyl-2-octen-1-one, B-70206
1-Bromo-(2-dimethoxymethyl)naphthalene, *in* B-60302
3-Bromo-2,6-dimethoxyphenol, *in* B-60200
4-Bromo-2,6-dimethoxyphenol, *in* B-60201
1-Bromo-3,3-dimethyl-1-butyne, B-70207
5-Bromo-3,3-dimethylcyclohexene, B-80199
1-Bromo-2,3-dimethylcyclopropene, B-60235
3-Bromo-2,2-dimethylpropanol, B-80200
4-Bromo-3,5-dimethylpyrazole, B-70208
3-Bromo-1,4-dimethylpyrazole, *in* B-70250
3-Bromo-1,5-dimethylpyrazole, *in* B-70252
4-Bromo-1,3-dimethylpyrazole, *in* B-70251
4-Bromo-1,5-dimethylpyrazole, *in* B-70251
5-Bromo-1,3-dimethylpyrazole, *in* B-70252
5-Bromo-4,6-dimethyl-1,2,3-triazine, B-80201
4-Bromodiphenylmethanol, B-60236
1-Bromo-1,2-diphenylpropene, B-60237
3-Bromo-1,2-diphenylpropene, B-70209
6′-Bromodisidein, *in* D-60499
Bromododecahedrane, B-80202
6-Bromo-6-dodecene, B-60238
2-Bromo-5,6-epoxy-4-hydroxy-2-cyclohexen-1-one, B-60239
1,1′,1″-(1-Bromo-1,2,2-ethenediyl)trisbenzene, *see* B-70276
5-(2-Bromoethenyl)-2′-deoxyuridine, *see* B-80266
1-(2-Bromoethenyl)-2,4,5-trichloro-1,5-dimethylcyclohexane, *see* T-80005
2-Bromo-3-ethoxy-1,4-naphthoquinone, *in* B-60268
2-Bromo-1-ethoxy-3-nitrobenzene, *in* B-70257
2-Bromo-3-ethoxypyridine, *in* B-60275
▷ 1-Bromoethyl phenyl ketone, *see* B-80243
2-(2-Bromoethyl)pyridine, B-70210
3-(2-Bromoethyl)pyridine, B-70211
5-Bromo-2-ethynylpyridine, B-80203
1β-Bromo-4(15)-eudesmen-11-ol, *see* B-60197
2-Bromo-3-fluoroanisole, *in* B-60247
2-Bromo-4-fluoroanisole, *in* B-60248
4-Bromo-2-fluoroanisole, *in* B-60251
3-Bromo-4-fluorobenzenemethanol, *see* B-60244
5-Bromo-2-fluorobenzenemethanol, *see* B-60245
2-Bromo-4-fluorobenzoic acid, B-60240
2-Bromo-5-fluorobenzoic acid, B-60241
2-Bromo-6-fluorobenzoic acid, B-60242
3-Bromo-4-fluorobenzoic acid, B-60243
3-Bromo-4-fluorobenzyl alcohol, B-60244
5-Bromo-2-fluorobenzyl alcohol, B-60245
1-Bromo-2-fluoro-3,5-dinitrobenzene, B-60246
2-Bromo-1-fluoro-3-methoxybenzene, *in* B-60247
2-Bromo-4-fluoro-1-methoxybenzene, *in* B-60248
4-Bromo-2-fluoro-1-methoxybenzene, *in* B-60251
2-Bromo-3-fluorophenol, B-60247
2-Bromo-4-fluorophenol, B-60248
2-Bromo-6-fluorophenol, B-60249
3-Bromo-4-fluorophenol, B-60250
4-Bromo-2-fluorophenol, B-60251
1-Bromo-3-fluoropropane, B-70212
2-Bromo-3-fluoropyridine, B-70213
2-Bromo-5-fluoropyridine, B-60252
3-Bromo-2-fluoropyridine, B-60253
3-Bromo-4-fluoropyridine, B-70214
3-Bromo-5-fluoropyridine, B-60254
4-Bromo-3-fluoropyridine, B-60255
5-Bromo-2-fluoropyridine, B-60256
▷ α-Bromo-*m*-fluorotoluene, *see* B-80216
▷ α-Bromo-*o*-fluorotoluene, *see* B-80215
▷ α-Bromo-*p*-fluorotoluene, *see* B-80217
3-Bromo-2-furancarboxaldehyde, B-60257
4-Bromo-2-furancarboxaldehyde, B-60258
5-Bromo-2-furancarboxaldehyde, B-60259
5-Bromo-2(5*H*)-furanone, B-80204
3-Bromofurfural, *see* B-60257
4-Bromofurfural, *see* B-60258
5-Bromofurfural, *see* B-60259
8-Bromoguanine, B-80205
8-Bromoguanosine, B-70215
▷ 1-Bromo-1,1,2,2,3,3,3-heptafluoropropane, B-80206
2-Bromo-1,1,1,2,3,3,3-heptafluoropropane, B-80207
6-Bromo-1-heptene, B-80208
7-Bromo-1-heptene, B-60260
7-Bromo-5-heptynoic acid, B-60261
1-Bromohexadecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene, *see* B-80202
2-Bromo-1,5-hexadiene, B-70216
5-Bromo-2-hexanone, B-60262
1-Bromo-3-hexene, B-80209
5-Bromo-1-hexene, B-60263
6-Bromo-1-hexene, B-60264
α-(1-Bromo-3-hexenyl)-5-(1-bromo-2-propynyl)tetrahydro-3-hydroxy-2-furanethanol, B-70217
1-Bromo-1-hexyne, B-70218
1-Bromo-2-hexyne, B-70219
5′-Bromo-2′-hydroxyacetophenone, B-60265
3-Bromo-5-hydroxy-2-methyl-1,4-naphthalenedione, *see* B-60266
3-Bromo-5-hydroxy-2-methyl-1,4-naphthoquinone, B-60266
2-Bromo-3-hydroxy-6-methylpyridine, B-60267
2-Bromo-3-hydroxy-1,4-naphthalenedione, *see* B-60268
2-Bromo-5-hydroxy-1,4-naphthalenedione, *see* B-60269
2-Bromo-6-hydroxy-1,4-naphthalenedione, *see* B-60270
2-Bromo-8-hydroxy-1,4-naphthalenedione, *see* B-60272
7-Bromo-2-hydroxy-1,4-naphthalenedione, *see* B-60273
8-Bromo-2-hydroxy-1,4-naphthalenedione, *see* B-60274
2-Bromo-3-hydroxy-1,4-naphthoquinone, B-60268
2-Bromo-5-hydroxy-1,4-naphthoquinone, B-60269
2-Bromo-6-hydroxy-1,4-naphthoquinone, B-60270
2-Bromo-7-hydroxy-1,4-naphthoquinone, B-60271
2-Bromo-8-hydroxy-1,4-naphthoquinone, B-60272
7-Bromo-2-hydroxy-1,4-naphthoquinone, B-60273
8-Bromo-2-hydroxy-1,4-naphthoquinone, B-60274
3-Bromo-5-hydroxy-7-oxabicyclo[4.1.0]hept-3-en-2-one, *see* B-60239
1-(5-Bromo-2-hydroxyphenyl)ethanone, *see* B-60265
6-Bromo-5-hydroxy-2-picoline, *see* B-60267
▷ 2-Bromo-3-hydroxypyridine, B-60275
2-Bromo-5-hydroxypyridine, B-60276
3-Bromo-5-hydroxypyridine, B-60277
4-Bromo-3-hydroxypyridine, B-60278
▷ 2-Bromo-1*H*-imidazole, B-70220
4(5)-Bromo-1*H*-imidazole, B-70221
2-Bromoinosine, *see* B-70269
8-Bromoinosine, *see* B-70270
5-Bromo-2-iodoaniline, B-60279
5-Bromo-2-iodobenzenamine, *see* B-60279
1-Bromo-2-iodo-3-nitrobenzene, B-70222
2-Bromo-1-iodo-3-nitrobenzene, B-70223
2-Bromo-4-iodopyridine, B-60280
2-Bromo-5-iodopyridine, B-60281
3-Bromo-4-iodopyridine, B-60282
3-Bromo-5-iodopyridine, B-60283
4-Bromo-2-iodopyridine, B-60284
4-Bromo-3-iodopyridine, B-60285
5-Bromo-2-iodopyridine, B-60286
2-Bromo-4-iodothiazole, B-60287
2-Bromo-5-iodothiazole, B-60288
4-Bromo-2-iodothiazole, B-60289
5-Bromo-2-iodothiazole, B-60290
4-Bromo-1(3*H*)-isobenzofuranone, B-70224
7-Bromo-1(3*H*)-isobenzofuranone, B-70225
2-Bromoisobutyric acid, *see* B-80229
α-Bromoisobutyronitrile, *in* B-80229
1-Bromo-5-isopropylcyclopentene, B-80210
3-Bromo-5-isoxazolemethanamine, *see* A-70165
2-Bromojuglone, *see* B-60269
3-Bromojuglone, *see* B-60272
ent-3β-Bromo-13(16)-labdene-8β,14,15-triol, *see* V-70004
9-Bromolaurenisol, B-80211
2-Bromo-4-mercaptobenzoic acid, B-70226
2-Bromo-5-mercaptobenzoic acid, B-70227
3-Bromo-4-mercaptobenzoic acid, B-70228
3-Bromo-2-mercaptopyridine, *in* B-60315
2-Bromo-6-mercaptopyridine, *see* B-80256
3-Bromo-4-mercaptopyridine, *see* B-60316
5-Bromo-2-mercaptopyridine, *see* B-60317
3-Bromomesitoic acid, *see* B-60331
Bromomethanesulfonic acid, B-60291
Bromomethanol, B-80212
5′-Bromo-2′-methoxyacetophenone, *in* B-60265
2-Bromo-3-methoxyaniline, *in* A-70099
2-Bromo-3-methoxy-2-cyclohexen-1-one, *in* B-70201
2-Bromo-3-methoxy-6-methylpyridine, *in* B-60267
2-Bromo-6-methoxy-1,4-naphthaquinone, *in* B-60270
2-Bromo-3-methoxy-1,4-naphthoquinone, *in* B-60268
2-Bromo-5-methoxy-1,4-naphthoquinone, *in* B-60269
2-Bromo-7-methoxy-1,4-naphthoquinone, *in* B-60271
2-Bromo-8-methoxy-1,4-naphthoquinone, *in* B-60272
2-Bromo-1-methoxy-3-nitrobenzene, *in* B-70257
1-(5-Bromo-2-methoxyphenyl)ethanone, *in* B-60265
6-Bromo-5-methoxy-2-picoline, *in* B-60267
2-Bromo-3-methoxypyridine, *in* B-60275
3-Bromo-5-methoxypyridine, *in* B-60277
1-(Bromomethyl)acridine, B-70229
2-(Bromomethyl)acridine, B-70230
3-(Bromomethyl)acridine, B-70231

4-(Bromomethyl)acridine, B-70232
9-(Bromomethyl)acridine, B-70233
α-Bromomethylacrylic acid, *see* B-70249
2-Bromo-3-methylaniline, B-70234
2-Bromo-3-methylbenzaldehyde, B-60292
2-Bromo-3-methylbenzenamine, *see* B-70234
2-Bromo-3-methylbenzoic acid, B-60293
3-Bromo-4-methylbenzoic acid, B-60294
3-Bromo-3-methyl-1-butyne, B-80213
2-(Bromomethyl)-6-chloropyridine, B-70235
3-(Bromomethyl)-2-chloropyridine, B-70236
4-(Bromomethyl)-2-chloropyridine, B-70237
5-(Bromomethyl)-2-chloropyridine, B-70238
2-(Bromomethyl)cyclohexanamine, B-70239
2-(Bromomethyl)cyclopentanamine, B-70240
(Bromomethyl)cyclopentane, B-70241
1-Bromo-1-methylcyclopropane, B-70242
1,1′-[3-(Bromomethyl)-1,2-cyclopropanediyl]bisbenzene, *see* B-80214
3-(Bromomethyl)-2,3-dihydrobenzofuran, B-60295
1-Bromomethyl-2,3-diphenylcyclopropane, B-80214
3-Bromo-2-methylenepropanoic acid, *see* B-70249
(Bromomethylene)tricyclo[3.3.1.1^{3,7}]decane, *see* B-60296
1,1′-[1-(Bromomethyl)-1,2-ethenediyl]bisbenzene, *see* B-70209
1,1′-(1-Bromo-2-methyl-1,2-ethenediyl)bisbenzene, *see* B-60237
1-Bromo-5-(1-methylethyl)cyclopentene, *see* B-80210
▷ 1-(Bromomethyl)-2-fluorobenzene, B-80215
▷ 1-(Bromomethyl)-3-fluorobenzene, B-80216
▷ 1-(Bromomethyl)-4-fluorobenzene, B-80217
2-(Bromomethyl)-6-fluoropyridine, B-70243
3-(Bromomethyl)-2-fluoropyridine, B-70244
4-(Bromomethyl)-2-fluoropyridine, B-70245
5-(Bromomethyl)-2-fluoropyridine, B-70246
(Bromomethylidene)adamantane, B-60296
4-Bromo-1-methyl-1*H*-imidazole, *in* B-70221
5-Bromo-1-methyl-1*H*-imidazole, *in* B-70221
Bromomethyl isobutyl ketone, *see* B-60298
3-Bromo-5-methylisoquinoline, B-80218
4-Bromo-1-methylisoquinoline, B-80219
5-Bromo-3-methylisoquinoline, B-80220
5-(Bromomethyl)isoxazole, B-80221
5-Bromomethyl-2-(4-methyl-1,4-cyclohexadienyl)-2-methyl-1-methylenecyclopentane, *see* B-70247
3-(Bromomethyl)-1-methyl-2-methylene-1-(4-bromophenyl)cyclopentane, *in* B-70247
1-[3-(Bromomethyl)-1-methyl-2-methylenecyclopentyl]-4-methylbenzene, *in* B-70247
1-[3-(Bromomethyl)-1-methyl-2-methylenecyclopentyl]-4-methyl-1,4-cyclohexadiene, B-70247
4-(Bromomethyl)-2-nitrobenzoic acid, B-60297
▷ (Bromomethyl)pentafluorobenzene, B-80222
1-Bromo-3-methylpentane, B-80223
2-Bromo-4-methylpentanoic acid, B-70248
1-Bromo-4-methyl-2-pentanone, B-60298
5-Bromo-3-methyl-1-pentene, B-60299
1-(Bromomethyl)phenanthrene, B-80224
2-(Bromomethyl)phenanthrene, B-80225
3-(Bromomethyl)phenanthrene, B-80226
9-(Bromomethyl)phenanthrene, B-80227
1-Bromo-2-methyl-1-phenylpropene, B-80228
Bromomethyl phenyl selenide, B-60300
▷ 2-Bromo-2-methylpropanoic acid, B-80229
2-Bromomethyl-2-propenoic acid, B-70249
(1-Bromo-2-methyl-1-propenyl)benzene, *see* B-80228
3(5)-Bromo-4-methylpyrazole, B-70250
3(5)-Bromo-5(3)-methylpyrazole, B-70252
4-Bromo-3(5)-methylpyrazole, B-70251
▷ 4-Bromo-1-methylpyrazole, *in* B-80254
2-(Bromomethyl)pyridine, B-70253
3-(Bromomethyl)pyridine, B-70254
4-(Bromomethyl)pyridine, B-70255
2-Bromo-6-methyl-3-pyridinol, *see* B-60267
4-Bromo-6-methylpyrimidine, B-80230
5-Bromo-4-methylpyrimidine, B-80231
[(Bromomethyl)seleno]benzene, *see* B-60300
2-Bromo-6-(methylsulfonyl)pyridine, *in* B-80256
5-Bromo-2-(methylsulfonyl)pyridine, *in* B-60317
2-Bromo-4-(methylthio)benzoic acid, *in* B-70226
2-Bromo-5-(methylthio)benzoic acid, *in* B-70227
3-Bromo-4-(methylthio)benzoic acid, *in* B-70228
2-Bromo-6-(methylthio)pyridine, *in* B-80256
3-Bromo-2-(methylthio)pyridine, *in* B-60315
5-Bromo-2-(methylthio)pyridine, *in* B-60317
4-Bromo-5-methyl-1,2,3-triazine, B-80232
5-Bromo-4-methyl-1,2,3-triazine, B-80233
3-(Bromomethyl)-2,4,10-trioxadamantane, *see* B-60301
(3-Bromomethyl)-2,4,10-trioxatricyclo[3.3.1.1^{3,7}]decane, B-60301
2-Bromo-4-methylvaleric acid, *see* B-70248
1-Bromo-2-naphthaldehyde, *see* B-60302
1-Bromo-2-naphthalenecarboxaldehyde, B-60302
1-(3-Bromo-1-naphthalenyl)ethanone, *see* A-60021
1-(4-Bromo-1-naphthalenyl)ethanone, *see* A-60022
1-(5-Bromo-1-naphthalenyl)ethanone, *see* A-60023
1-(6-Bromo-2-naphthalenyl)ethanone, *see* A-60025
1-(7-Bromo-1-naphthalenyl)ethanone, *see* A-60024
3-Bromo-1-naphthyl methyl ketone, *see* A-60021
4-Bromo-1-naphthyl methyl ketone, *see* A-60022
5-Bromo-1-naphthyl methyl ketone, *see* A-60023
6-Bromo-2-naphthyl methyl ketone, *see* A-60025
7-Bromo-1-naphthyl methyl ketone, *see* A-60024
2-Bromo-2-nitroadamantane, B-80234
2-Bromo-3-nitroanisole, *in* B-70257
4-Bromo-2-nitrobenzaldehyde, B-80235
4-Bromo-3-nitrobenzaldehyde, B-80236
▷ 5-Bromo-2-nitrobenzaldehyde, B-80237
2-Bromo-3-nitrobenzenemethanol, *see* B-70256
4-Bromo-2-nitrobenzenemethanol, *see* B-80238
2-Bromo-3-nitrobenzotrifluoride, *see* B-60308
2-Bromo-5-nitrobenzotrifluoride, *see* B-60307
3-Bromo-2-nitrobenzotrifluoride, *see* B-60306
5-Bromo-2-nitrobenzotrifluoride, *see* B-60309
2-Bromo-3-nitrobenzyl alcohol, B-70256
4-Bromo-2-nitrobenzyl alcohol, B-80238
1-Bromo-2-nitroethane, B-60303
2-Bromo-3-nitrophenetole, *in* B-70257
2-Bromo-3-nitrophenol, B-70257
1-Bromo-1-nitropropane, B-70258
2-Bromo-2-nitropropane, B-70259
3(5)-Bromo-5(3)-nitro-1*H*-pyrazole, B-60305
4-Bromo-3(5)-nitro-1*H*-pyrazole, B-60304
2-Bromo-4-nitrothiophene, B-80239
2-Bromo-2-nitrotricyclo[3.3.1.1^{3,7}]decane, *see* B-80234
1-Bromo-2-nitro-3-(trifluoromethyl)benzene, B-60306
1-Bromo-4-nitro-2-(trifluoromethyl)benzene, B-60307
2-Bromo-1-nitro-3-(trifluoromethyl)benzene, B-60308
4-Bromo-1-nitro-2-(trifluoromethyl)benzene, B-60309
2-Bromo-5-nitro-α,α,α-trifluorotoluene, *see* B-60307
1-Bromo-3-nonene, B-60310
2-Bromo-1-norbornanecarboxylic acid, *see* B-60210
8-Bromo-1-octanol, B-70260
1-Bromo-1-octene, B-70261
(3-Bromo-2-oxopropylidene)propanedioic acid, B-70262
15-Bromo-9(11)-parguerene-2,7,16,19-tetrol, B-80240
15-Bromo-9(11)-parguerene-2,7,16-triol, B-80241
1-Bromo-1,3-pentadiene, B-60311
Bromopentamethylbenzene, B-60312
5-Bromopentanal, B-70263
5-Bromo-2-pentanol, B-60313
2-Bromo-1,10-phenanthroline, B-70264
8-Bromo-1,7-phenanthroline, B-70265
4-Bromo-α-phenylbenzenemethanol, *see* B-60236
2-Bromo-4-phenylbenzoic acid, *see* B-60211
2-Bromo-4-phenylbutanoic acid, B-80242
3-Bromo-1-phenyl-1-butyne, B-60314
4-Bromophenylphenylmethanol, *see* B-60236
▷ 2-Bromo-1-phenyl-1-propanone, B-80243
3-Bromo-3-phenyl-1-propyne, B-80244
5-Bromo-1-phenylpyrazole, *in* B-80253
2-Bromo-4-phenylpyridine, B-80245
2-Bromo-5-phenylpyridine, B-80246
2-Bromo-6-phenylpyridine, B-80247
3-Bromo-2-phenylpyridine, B-80248
3-Bromo-4-phenylpyridine, B-80249
4-Bromo-2-phenylpyridine, B-80250
5-Bromo-2-phenylpyridine, B-80251
5-Bromo-4-phenyl-1,2,3-triazine, B-80252
2-Bromophloroglucinol, *see* B-60199
1-Bromophthalazine, B-70266
5-Bromophthalazine, B-70267
6-Bromophthalazine, B-70268
4-Bromophthalide, *see* B-70224
7-Bromophthalide, *see* B-70225
3-Bromoplumbagin, *see* B-60266
▷ 2-Bromopropiophenone, *see* B-80243
(1-Bromo-2-propynyl)benzene, *see* B-80244
3(5)-Bromopyrazole, B-80253
▷ 4-Bromopyrazole, B-80254
3-Bromo-2-pyridinethiol, *in* B-60315
3-Bromo-4-pyridinethiol, *see* B-60316
5-Bromo-2-pyridinethiol, *see* B-60317
6-Bromo-2-pyridinethiol, *see* B-80256
3-Bromo-2(1*H*)-pyridinethione, B-60315
3-Bromo-4(1*H*)-pyridinethione, B-60316
5-Bromo-2(1*H*)-pyridinethione, B-60317
6-Bromo-2(1*H*)-pyridinethione, B-80256
▷ 2-Bromo-3-pyridinol, *see* B-60275
4-Bromo-3-pyridinol, *see* B-60278
5-Bromo-3-pyridinol, *see* B-60277
6-Bromo-3-pyridinol, *see* B-60276
2-Bromo-5-pyrimidinamine, *see* A-70103
4-Bromo-2-pyrimidinamine, *see* A-70100
5-Bromo-2-pyrimidinamine, *see* A-70101
5-Bromo-4-pyrimidinamine, *see* A-70102
▷ 5-Bromo-2,4-(1*H*,3*H*)-pyrimidinedione, B-60318
6-Bromo-2,4-(1*H*,3*H*)-pyrimidinedione, B-60319
4-Bromopyrogallol, *see* B-60200
5-Bromopyrogallol, *see* B-60201
3-Bromo-2-pyrrolidinone, B-80258
8-Bromo-9-β-D-ribofuranosylguanine, *see* B-70215
2-Bromo-9-β-D-ribofuranosyl-6*H*-purin-6-one, B-70269
8-Bromo-9-β-D-ribofuranosyl-6*H*-purin-6-one, B-70270
4-Bromo-2-sulfolene, *in* B-70204
1-Bromo-2,3,4,5-tetrafluorobenzene, B-60320
2-Bromo-1,3,4,5-tetrafluorobenzene, B-60321
3-Bromo-1,2,4,5-tetrafluorobenzene, B-60322
1-Bromo-2,3,4,6-tetrafluorobenzene, *see* B-60321
1-Bromo-2,3,5,6-tetrafluorobenzene, *see* B-60322
1-Bromo-1,1,2,2-tetrafluoroethane, B-80259

1-Bromo-1,1,2,2-tetrafluoro-2-iodoethane, B-80260
1-Bromo-2,3,4,5-tetrafluoro-6-nitrobenzene, B-60323
1-Bromo-2,3,4,6-tetrafluoro-5-nitrobenzene, B-60324
1-Bromo-2,3,5,6-tetrafluoro-4-nitrobenzene, B-60325
2-Bromo-3,4,5,6-tetrafluoropyridine, B-60326
3-Bromo-2,4,5,6-tetrafluoropyridine, B-60327
4-Bromo-2,3,5,6-tetrafluoropyridine, B-60328
2-Bromotetrahydro-2*H*-pyran, B-70271
7-Bromo-1-tetralone, *see* B-60234
3-Bromo-1,1,2,2-tetramethylcyclopropane, B-80261
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5-Bromo-1*H*-tetrazole, B-80262
5-Bromo-4-thiouracil, *see* B-70205
Bromothricin, *in* C-60137
2-Bromo-*m*-toluic acid, *see* B-60293
3-Bromo-*p*-toluic acid, *see* B-60294
2-Bromo-*m*-toluidine, *see* B-70234
5-Bromo-1,2,3-triazine, B-70273
5-Bromo-1,2,3-triazine, B-80263
3-Bromo[1,2,3]triazolo[1,5-*a*]pyridine, B-60329
7-Bromo[1,2,3]triazolo[1,5-*a*]pyridine, B-60330
1-Bromo-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexane, B-70274
1-Bromo-2,3,3-trifluorocyclopropene, B-80264
2-Bromo-1,1,1-trifluoroethane, B-80265
▷ 3-Bromo-3-(trifluoromethyl)-3*H*-diazirine, B-70275
(Bromotrifluoromethyl)propiolic acid, *see* B-70202
2-Bromo-α,α,α-trifluoro-3-nitrotoluene, *see* B-60308
3-Bromo-α,α,α-trifluoro-2-nitrotoluene, *see* B-60306
5-Bromo-α,α,α-trifluoro-2-nitrotoluene, *see* B-60309
15-Bromo-2,7,16-trihydroxy-9(11)-parguerene, *see* B-80241
1-Bromo-2,3,4-trimethoxybenzene, *in* B-60200
1-Bromo-2,3,5-trimethoxybenzene, *in* B-70182
1-Bromo-2,4,5-trimethoxybenzene, *in* B-70181
2-Bromo-1,3,4-trimethoxybenzene, *in* B-70180
2-Bromo-1,3,5-trimethoxybenzene, *in* B-60199
5-Bromo-1,2,3-trimethoxybenzene, *in* B-60201
3-Bromo-2,4,6-trimethylbenzoic acid, B-60331
2-Bromo-1,1,9-trimethyl-5-methylenespiro[5.5]undeca-7,9-dien-3-ol, *see* I-70074
2-Bromo-1,1,9-trimethylspiro[5.5]undeca-7,9-dien-3-ol, *see* O-70001
Bromotriphenylethylene, B-70276
2-Bromotryptophan, B-60332
5-Bromotryptophan, B-60333
6-Bromotryptophan, B-60334
7-Bromotryptophan, B-60335
11-Bromo-1-undecene, B-60336
1-Bromo-2-undecene, B-70277
▷ 5-Bromouracil, *see* B-60318
6-Bromouracil, *see* B-60319
δ-Bromovaleraldehyde, *see* B-70263
5-(2-Bromovinyl)-2′-deoxyuridine, B-80266
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Bryoflavone, B-70283
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1,3-Butadiene-2,3-dicarboxylic acid, *see* D-70409
4*a*,8*a*-[1,3]Butadienonaphthalene, *see* T-70232
6-(1,3-Butadienyl)-1,4-cycloheptadiene, B-70290
2-(1,3-Butadienyl)-3-(1,3,5-heptatriynyl)oxirane, B-80277
1,1′-(1,3-Butadienylidene)bisbenzene, *see* D-70476
1,3-Butadienyl thiocyanate, *see* T-60210
1,1′,1″-(1,3-Butadien-1-yl-4-ylidene)trisbenzene, *see* T-70305
1,3-Butadiynylbenzene, *see* P-80095
1,3-Butanedithiol, B-60339
2,2-Butanedithiol, B-60340
6α-Butanoyloxy-17β-hydroxy-15,17-oxido-16-spongianone, *in* D-60365
Butein, *see* D-80362
▷ 2-Buten-1-amine, B-80278
3-Butene-1,2-diol, B-70291
2-Butene-1,4-dithiol, B-70292
2-Butene-1,4-diyl dithiocyanate, *see* D-60510
▷ 1-Butene oxide, *see* E-70047
3-Butenophenone, *see* P-60085
α-3-Butenylbenzenemethanamine, *see* A-70183
4-(2-Butenyl)-4-methylthreonine, *see* A-60189
5′-(3-Buten-1-ynyl)-[2,2′-bithienyl]-2-methanol, *see* B-80279
3-Buten-1-ynylcyclopropane, B-70293
5-(3-Buten-1-ynyl)-5′ hydroxymethyl-2,2′-bithienyl, B-80279
5-(3-Buten-1-ynyl)-5′-methyl-2,2′-bithienyl, *in* B-80279
2-(3-Buten-1-ynyl)-5-(1,3-pentadiynyl)thiophene, B-80280
2-(3-Buten-1-ynyl)-5-(3-penten-1-ynyl)thiophene, *in* B-80280
5-[5-(3-Buten-1-ynyl)-2-thienyl]-2-penten-4-ynal, *in* B-80281
5-[5-(3-Buten-1-ynyl)-2-thienyl]-2-penten-4-yn-1-ol, B-80281
Butoflin, *see* D-80027
Butox, *see* D-80027
tert-Butoxyethyne, *in* E-80070
1-*tert*-Butoxy-1-hexyne, B-80282
2-*tert*-Butoxysuccinic anhydride, *in* D-80211
3-Butylaspartic acid, *see* A-60102
3-*tert*-Butylbicyclo[3.1.0]hexane, B-70294
1-*tert*-Butyl-3-(*tert*-butylamino)-1*H*-pyrrole, *in* A-80143
tert-Butyl chloromethyl ether, B-70295
3-*tert*-Butyl-2-cyclobuten-1-one, B-80283
1-*tert*-Butyl-1,3-cyclohexadiene, B-70296
1-*tert*-Butylcyclohexene, B-60341
3-*tert*-Butylcyclohexene, B-60342
4-*tert*-Butylcyclohexene, B-60343
3-*tert*-Butyl-2-cyclohexen-1-one, B-70297
1-*tert*-Butyl-1,2-cyclooctadiene, B-60344
6-*tert*-Butylcyclopenta[*c*]pyran, B-80284
1-*tert*-Butylcyclopentene, B-70298
3-*tert*-Butylcyclopentene, B-70299
4-*tert*-Butylcyclopentene, B-70300
4-*tert*-Butylcyclopentene-1,2-oxide, *see* B-70294
tert-Butylcyclopropane, B-80285
1,1-*tert*-Butyl-3,3-diethoxy-2-azaallenium(1+), B-70301
2-*tert*-Butyl-2,4-dihydro-6-methyl-1,3-dioxol-4-one, B-60345
3-*tert*-Butyl-1,4,2-dioxazol-5-one, B-80286
5-*tert*-Butyl-1,2,3,5-dithiadiazolyl, B-70302
5-*tert*-Butyl-1,3,2,4-dithiadiazolyl, B-70303
sec-Butyl ethyl ketone, *see* M-80097
tert-Butylethynylcarbinol, *see* D-80468
2-*tert*-Butylglutaric acid, *see* B-80289
2-*tert*-Butylglutarimide, *in* B-80289
tert-Butylglycine, *see* A-70136
3-*sec*-Butylhexahydropyrrolo[1,2-*a*]pyrazine-1,4-dione, *see* H-60052
3-*tert*-Butyl-4-hydroxybenzaldehyde, B-70304
tert-Butyl hypoiodite, B-80287
3-Butylidene-4,5-dihydro-1(3*H*)-isobenzofuranone, *see* L-60026
3-Butylidene-4,5-dihydrophthalide, *see* L-60026
4-(Butylimino)-3,4-dihydro-1,2,3-benzotriazine(incorr.), *in* A-60092
▷ 2-*tert*-Butylimino-3-isopropyl-5-phenyl-1,3,5-thiadiazinan-4-one, *see* B-80276
Butyliodoacetylene, *see* I-70040
1-*tert*-Butyl-2-iodobenzene, B-60346
1-*tert*-Butyl-3-iodobenzene, B-60347
1-*tert*-Butyl-4-iodobenzene, B-60348
tert-Butyl iodomethyl ketone, *see* I-60044
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▷ Butyl isocyanide, *see* I-80058
tert-Butyl isopropyl ketone, *see* T-60366
▷ *tert*-Butyl isothiocyanate, *see* I-70105
2-*tert*-Butyllactic acid, *see* H-80262
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tert-Butylmethylacetylene, *see* D-60438
2-*tert*-Butyl-6-methyl-1,3-dioxan-4-one, *see* B-60345
▷ *tert*-Butyl mustard oil, *see* I-70105
4-*tert*-Butyl-2(3*H*)-oxazolethione, B-80288
S-Butyl 3-oxobutanethioate, *in* O-70080
S-*tert*-Butyl 3-oxobutanethioate, *in* O-70080
2-*tert*-Butylpentanedioic acid, B-80289
2-*tert*-Butylphenanthrene, B-70305
3-*tert*-Butylphenanthrene, B-70306
9-*tert*-Butylphenanthrene, B-70307
tert-Butylphenylacetylene, *see* D-60441
tert-Butyl phenyl ketone, *see* D-60443
3-*tert*-Butyl-2,6-piperidinedione, *in* B-80289
tert-Butyl-1-propenyl ketone, *see* D-70414
3(5)-*tert*-Butylpyrazole, B-80291
4-*tert*-Butylpyrazole, B-80292
2-*tert*-Butyl-4(3*H*)-pyrimidinone, B-60349
sec-Butylsuccinic acid, *see* M-80150
tert-Butylsulfinic acid, B-80293
3-*tert*-Butyl-2,2,4,5,5-tetramethyl-3-hexene, B-60350
2-*sec*-Butyl-2-thiazoline, *see* D-70224
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2-Butynedial, B-60351
2-Butyne-1,4-dithiol, B-70308
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▷ C.I. Basic Violet 14, *see* R-60010
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▷ C.I. Disperse Red 15, *see* A-60175
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C.I. Mordant Violet 39, *in* A-60318
C.I. Pigment Yellow 24, *see* F-80010
▷ C.I. Solvent Red 53, *see* A-60175
C.I. Vat Yellow 1, *see* F-80010
C_2-Bishomocuban-6-one, *see* P-60027
Cabreuvin, *in* T-80308
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14-Cadalenal, *see* I-80084
Cadambagenic acid, C-70002
4(15),5-Cadinadiene, C-70003
4(14),10(15)-Cadinadiene, *see* C-60001
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4,11(13)-Cadinadien-12-oic acid, C-70004
1,9-Cadinadien-3-one, C-80003
4,6,11(13)-Cadinatrien-12-oic acid, *in* C-70004
ε-Cadinene, C-60001
4-Cadinene-1-isothiocyanate, *see* I-80094
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4-*O*-Cadinylangolensin, C-80004
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Caespitane, *in* C-80005
Caespitol, C-80005
▷ Cafaloin, *see* B-80010
Caffeidine, C-60003
3-*O*-[6-*O*-(2,5-di-*O*-Caffeoyl-α-L-arabinofuranosyl)-β-D-glucopyranosyl]-3′,7-di-*O*-(6-*O*-caffeoyl-β-D-glucopyranosyl)cyanidin, *see* Z-70002
▷ 3-*O*-Caffeoylquinic acid, C-70005
4-*O*-Caffeoylshikimic acid, C-80006
5-*O*-Caffeoylshikimic acid, C-80007
3-*O*-Caffeoyl-4-O-sinapoylquinic acid, *in* C-70005
▷ Caffetannic acid, *see* C-70005
▷ Caffeylquinic acid, *see* C-70005
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N-Carbamoylglucosamine, C-70015
N^6-(Carbamoylmethyl)-2′-deoxyadenosine, C-70016
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Carbapenam-3-carboxylic acid, *see* O-70079
9*H*-Carbazole-1,8-diamine, *see* D-80056
1*H*-Carbazole-1,4(9*H*)-dione, C-60012
9*H*-Carbazol-2-ol, *see* H-60109
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1,1′-Carbonothioylbis-2(1*H*)pyridinone, C-60014
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O,*O*′-Carbonylbis(hydroxylamine), C-60015
N,*N*′-[Carbonylbis(oxy)]bis[2-methyl-2-propanamine], *in* C-60015
3,3′-Carbonylbis[5-phenyl-1,3,4-oxadiazole-2(3*H*)-thione], C-80021
2,2′-Carbonyldibenzoic acid, *see* B-70041
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2-Carboxycyclohexaneacetic acid, C-80023
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5-Carboxydecahydro-β-5,8*a*-trimethyl-2-methylene-1-naphthalenepentanoic acid, *see* O-60039
3-Carboxy-2,3-dihydro-8-hydroxy-5-methylthiazolo[3,2-*a*]pyridinium hydroxide inner salt, C-70021
2-Carboxy-1,1-dimethylpyrrolidinium hydroxide inner salt, *see* S-60050
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4-(2-Carboxyethyl)-4-nitroheptanedioic acid, C-80025
N^2-(1-Carboxyethyl)ornithine, *see* O-80023
2-Carboxy-3-fluorobenzenethiol, *see* F-70030
2-Carboxy-5-fluorobenzenethiol, *see* F-70031
4-Carboxy-3-fluorobenzenethiol, *see* F-70029
17-Carboxygrindelic acid, *see* E-70024
5-Carboxy-α-hydroxy-2-furanacetic acid, *see* O-70048
N-(*N*-1-Carboxy-6-hydroxy-3-oxoheptyl)alanyltyrosine, C-70022
5-[(3-Carboxy-4-hydroxyphenyl)(3-carboxy-4-oxo-2,5-cyclohexadien-1-ylidene)methyl]-2-hydroxybenzoic acid, *see* A-60318
3-Carboxy-2-hydroxy-*N*,*N*,*N*-trimethyl-1-propanaminium hydroxide inner salt, *see* C-70024
(1-Carboxy-2-imidazol-4-ylethyl)trimethylammonium hydroxide inner salt, *see* H-60083
4-Carboxy-2-iodobenzenethiol, *see* I-70046
4-Carboxy-3-methoxy-5-pentylphenyl 2,4-dimethoxy-6-pentylbenzoate, *see* P-80158
N-(Carboxymethyl)-β-alanine, *see* C-60016
3-(Carboxymethylamino)propanoic acid, C-60016
▷ 3-(Carboxymethylamino)propionitrile, *in* C-60016
5-(Carboxymethyl)decahydro-1,5,8*a*-trimethyl-2,6-dioxo-1-naphthalenepropanoic acid, *see* O-80071
▷ 2-Carboxy-4-(1-methylethenyl)-3-pyrrolidineacetic acid, *see* K-60003
3-Carboxy-4-methylhexanoic acid, *see* M-80150
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▷ 3-Carboxymethyl-4-isopropenylproline, *see* K-60003
4-Carboxy-3-nitrobenzyl bromide, *see* B-60297
1-(2-Carboxy-5-oxo-1-pyrrolidinyl)-1-deoxy-D-mannitol, *see* A-70075
2-Carboxyphenothiazine, *see* P-70056
9-(2-Carboxyphenyl)-3,6-bis(diethylamino)xanthylium, *see* R-80006
[9-(*o*-Carboxyphenyl)-6-(diethylamino)-3*H*-xanthen-3-ylidene]diethylammonium, *see* R-80006
N-[[9-(2-Carboxyphenyl)-6-diethylamino]-3*H*-xanthen-3-ylidene]-*N*-ethyl ethanaminium, *see* R-80006
S-(2-Carboxypropyl)cysteine, *see* I-80049
3-[(2-Carboxypropyl)sulfonyl]alanine, *in* I-80049
3-[(2-Carboxypropyl)thio]alanine, *see* I-80049
5-Carboxyprotocatechuic acid, *see* D-60307
2-Carboxy-3-thiopheneacetic acid, C-60017
4-Carboxy-3-thiopheneacetic acid, C-60018
α-Carboxy-*N*,*N*,*N*-trimethyl-1*H*-imidazole-4-ethanaminium hydroxide inner salt, *see* H-60083
▷ Carbyloxime, *see* F-80086
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Carnosiflogenin *B*, *in* C-60175
Carnosiflogenin *C*, *in* C-60175
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Carnosifloside II, *in* C-60175
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ψ,ψ-Carotene, *see* L-60041
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1,3,7,11-Cembratetraen-15-ol, C-70029
3,7,11,15(17)-Cembratetraen-16,2-olide, C-60028
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Chiriquixanthin A, *in* T-80370
Chiriquixanthin B, *in* T-80370
Chiriquixanthin B, *in* T-80370
Chisocheton compound *A*, *in* T-60223
Chisocheton compound *D*, *in* T-60223
Chlamydocin, C-60038
Chloramine T, *in* C-80071
Chloratranol, *see* C-60059
Chloretyl, *see* H-70053
▷ Chlorisept, *see* C-70075
4-Chloro-6-formylorcinol, *see* C-60060
4-Chloro-9*R*-*hydroxy*-3,7(14)-*chamigradiene*, *in* E-70002
2-(3-Chloro-4-acetoxy-1-butynyl)-5-(1,3-pentadiynyl)thiophene, *in* P-80025
2-Chloroacetyl-3-methylaniline, *see* A-60115
2-Chloroacetyl-4-methylaniline, *see* A-60114
2-Chloroacetyl-5-methylaniline, *see* A-60113
2-Chloroacetyl-6-methylaniline, *see* A-60112
1-Chloroadamantane, C-60039
2-Chloroadamantane, C-60040
2-Chloroadenine, *see* C-70039
2-Chloroallylamine, *see* C-70151
2-Chloro-6-aminopurine, C-70039
2-Chloro-1,4,9,10-anthracenetetrone, C-60041
3-Chloroaspartic acid, *see* A-70121
Chloroatranol, *see* C-60059
5-Chloro-6-azauracil, *see* C-80114
10-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70047
11-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70048
2-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70040
3-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70041
4-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70042
5-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70043
6-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70044
8-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70045
9-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70046
10-Chlorobenzanthrone, *see* C-70047
11-Chlorobenzanthrone, *see* C-70048
2-Chlorobenzanthrone, *see* C-70040
3-Chlorobenzanthrone, *see* C-70041
4-Chlorobenzanthrone, *see* C-70042
5-Chlorobenzanthrone, *see* C-70043
6-Chlorobenzanthrone, *see* C-70044
8-Chlorobenzanthrone, *see* C-70045
9-Chlorobenzanthrone, *see* C-70046
13-Chlorobenzanthrone (obsol.), *see* C-70041
2-Chlorobenzanthrone (obsol.), *see* C-70042
2′-Chlorobenzanthrone (obsol.), *see* C-70040
6-Chlorobenzanthrone (obsol.), *see* C-70046
7-Chlorobenzanthrone (obsol.), *see* C-70047
β-Chlorobenzeneethanol, *see* C-60128
p-Chlorobenzhydrol, *see* C-60065
4-Chloro-1,2-benzisothiazole, C-70050
5-Chloro-1,2-benzisothiazole, C-70051
6-Chloro-1,2-benzisothiazole, C-70052
7-Chloro-1,2-benzisothiazole, C-70053
1-Chlorobenzo[*a*]carbazole, C-80039
1-Chlorobenzo[*g*]phthalazine, C-70054
4-Chlorobenzo[*g*]phthalazin-1(2*H*)-one, C-70055
2-Chlorobenzo[*b*]thiophene, C-60042
3-Chlorobenzo[*b*]thiophene, C-60043
4-Chlorobenzo[*b*]thiophene, C-60044
5-Chlorobenzo[*b*]thiophene, C-60045
6-Chlorobenzo[*b*]thiophene, C-60046
7-Chlorobenzo[*b*]thiophene, C-60047
▷ 2-Chlorobenzoxazole, C-60048
2-Chlorobicyclo[2.2.1]hepta-2,5-diene, C-70056
1-Chlorobicyclo[2.2.2]octane, C-70057
2-Chloro-1,4-butanediol, C-80040
4-Chloro-2-buten-1-amine, C-50094
3-Chloro-1-butene, C-80042
2-Chloro-2-butenedioic acid, C-80043
4-Chloro-1-butyne, C-70058
4-Chloro-2-butyn-1-ol, C-80044
3-Chlorobutyrine, *see* A-60103
4-Chlorobutyrine, *see* A-60104
1′-(Chlorocarbonyl)-1′,2′-dihydro-1,2′-bipyridinium (1+), C-80045
2[(Chlorocarbonyl)oxy]-3*a*,4,7,7*a*-tetrahydro-4,7-methano-1*H*-isoindole-1,3(2*H*)-dione, C-70059
6-Chloro-3-(3-chloro-4-hydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* D-80147
1-Chloro-3-(chloromethyl)-7-methyl-2,6-octadiene, C-70060
3-Chloro-2-chloromethyl-1-propene, C-70061
α-Chloro-*m*-cresol, *see* C-70102
α-Chloro-*o*-cresol, *see* C-70101
α-Chloro-*p*-cresol, *see* C-70103
2-Chloro-6-cyanobenzenethiol, *in* C-70083
2-Chloro-4-cyanophenol, *in* C-60091
5-Chloro-1,3-cycloheptadiene, C-70062
2-Chloro-2-cyclohepten-1-one, C-60049
2-Chloro-1,3-cyclohexanedione, C-80046
2-Chloro-2-cyclohexen-1-one, C-60050
2-Chloro-2-cyclopenten-1-one, C-60051
5-Chloro-2-cyclopenten-1-one, C-70063
5′-Chloro-5′-deoxyarabinosylcytosine, C-70064
6-Chlorodibenzo[*c*,*g*]carbazole, C-80047
2-Chloro-1,2-dibromo-1,1,2-trifluoroethane, *see* D-80085
1-Chloro-1,2-dicyanoethylene, *in* C-80043
1-Chloro-1,2-difluoroethene, C-80048
▷ 2-Chloro-1,1-difluoroethene, C-80049
2-Chloro-4,6-difluoro-1,3,5-triazine, C-60052
6-Chloro-3,5-difluoro-1,2,4-triazine, C-60053
5-Chloro-5,6-dihydro-3,4-epoxy-2-(2,4,6-octatriynylidene)-2*H*-pyran, *in* C-80051
2-Chloro-4,5-dihydro-1*H*-imidazole, C-80050
2-Chloro-2,3-dihydro-1*H*-imidazole-4,5-dione, C-60054
4-Chloro-2,3-dihydro-1*H*-indole, C-60055
5-Chloro-5,6-dihydro-2-(2,4,6-octatriynylidene)-2*H*-pyran, C-80051
2-Chloro-3,6-dihydroxybenzaldehyde, C-60056
3-Chloro-2,5-dihydroxybenzaldehyde, C-60057
3-Chloro-2,6-dihydroxybenzaldehyde, C-60058
5-Chloro-2,3-dihydroxybenzaldehyde, C-70065
6-Chloro-5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* C-80120
2-Chloro-1,8-dihydroxy-5-methoxy-6-methylxanthone, *in* T-70181
3-Chloro-2,6-dihydroxy-4-methylbenzaldehyde, C-60059
3-Chloro-4,6-dihydroxy-2-methylbenzaldehyde, C-60060

2-Chloro-4,6-dihydroxypyridine, *see* C-70074
4-Chloro-2,6-dihydroxypyridine, *see* C-70073
2-Chloro-4,6-dihydroxy-1,3,5-triazine, *see* C-80115
6-Chloro-3,5-dihydroxy-1,2,4-triazine, *see* C-80114
5-Chloro-2,3-dimethoxybenzaldehyde, *in* C-70065
6-Chloro-2,3-dimethoxy-1,4-naphthalenediol diacetate, *in* C-60118
2-Chloro-4,6-dimethoxypyridine, *in* C-70074
4-Chloro-2,6-dimethoxypyridine, *in* C-70073
2-Chloro-4,6-dimethoxy-1,3,5-triazine, *in* C-80115
2-Chloro-4,6-dimethylbenzaldehyde, C-60061
4-Chloro-2,6-dimethylbenzaldehyde, C-60062
4-Chloro-3,5-dimethylbenzaldehyde, C-60063
5-Chloro-2,4-dimethylbenzaldehyde, C-60064
5-Chloro-4,6-dimethyl-1,2,3-triazine, C-80052
▷ 2-Chloro-1,3-dinitro-5-(trifluoromethyl)benzene, C-80053
4-Chlorodiphenylmethanol, C-60065
5-Chloro-4,6-diphenyl-1,2,3-triazine, C-80054
6′-Chlorodisidein, *in* D-60499
Chlorododecahedrane, C-80055
12-Chlorododecanoic acid, C-70066
2-Chloro-3,7-epoxy-9-chamigranone, C-60066
1-Chloro-9,10-epoxy-4,6-heptadecadiyne-2,3-diol, *in* P-80006
Chloroepoxytrifluoroethane, *see* C-60140
4-Chloro-2-ethoxy-1-nitrobenzene, *in* C-60119
(1-Chloroethyl) ethyl carbonate, C-60067
▷ 2-Chloroethyl isocyanate, *see* C-80069
▷ 2-Chloroethyl isothiocyanate, *see* C-70081
▷ β-Chloroethyl mustard oil, *see* C-70081
1-Chloro-1-ethynylcyclopropane, C-60068
2-Chloro-4-fluoroanisole, *in* C-60073
2-Chloro-5-fluoroanisole, *in* C-60074
4-Chloro-2-fluoroanisole, *in* C-60079
4-Chloro-3-fluoroanisole, *in* C-60080
3-Chloro-4-fluorobenzaldehyde, C-70067
3-Chloro-4-fluorobenzenethiol, C-60069
4-Chloro-2-fluorobenzenethiol, C-60070
4-Chloro-3-fluorobenzenethiol, C-60071
Chlorofluoroiodomethane, C-80056
1-Chloro-2-fluoro-4-mercaptobenzene, *see* C-60071
2-Chloro-1-fluoro-4-mercaptobenzene, *see* C-60069
4-Chloro-2-fluoro-1-mercaptobenzene, *see* C-60070
1-Chloro-2-fluoro-4-methoxybenzene, *in* C-60080
1-Chloro-4-fluoro-2-methoxybenzene, *in* C-60074
2-Chloro-4-fluoro-1-methoxybenzene, *in* C-60073
4-Chloro-2-fluoro-1-methoxybenzene, *in* C-60079
2-Chloro-4-fluoro-5-nitrobenzoic acid, C-60072
2-Chloro-4-fluorophenol, C-60073
2-Chloro-5-fluorophenol, C-60074
2-Chloro-6-fluorophenol, C-60075
3-Chloro-2-fluorophenol, C-60076
▷ 3-Chloro-4-fluorophenol, C-60077
3-Chloro-5-fluorophenol, C-60078
4-Chloro-2-fluorophenol, C-60079
4-Chloro-3-fluorophenol, C-60080
2-Chloro-3-fluoropyridine, C-60081
2-Chloro-4-fluoropyridine, C-60082
2-Chloro-5-fluoropyridine, C-60083
2-Chloro-6-fluoropyridine, C-60084
3-Chloro-2-fluoropyridine, C-60085
4-Chloro-2-fluoropyridine, C-60086
4-Chloro-3-fluoropyridine, C-60087
5-Chloro-2-fluoropyridine, C-60088
3-Chloro-4-fluorothiophenol, *see* C-60069
4-Chloro-2-fluorothiophenol, *see* C-60070
4-Chloro-3-fluorothiophenol, *see* C-60071
▷ Chloroflurazole, *see* D-60157
1-[2-(Chloroformyl)-2-azacyclohexa-3,5-dienyl]pyridinium, *see* C-80045
▷ Chlorofumaric acid, *in* C-80043
3-Chloro-2,5-furandione, *in* C-80043
▷ Chlorogenic acid, *see* C-70005
6-Chlorogenistein, *see* C-80120
3-Chlorogentisaldehyde, *see* C-60057
6-Chlorogentisaldehyde, *see* C-60056
8-Chloroguanine, C-80057
8-Chloroguanosine, C-70068
7-Chloro-2-heptenoic acid, C-70069
1-Chlorohexadecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene, *see* C-80055
2-Chloro-1,5-hexadiene, C-70070
6-Chloro-1-hexene, C-80058
2-Chloro-1-hexen-3-ol, C-80059
2-Chloro-4-hexen-3-ol, C-80060
4-Chloro-4-hexen-3-ol, C-80061
6-Chloro-2-hexen-1-ol, C-80062
6-Chloro-3-hexen-1-ol, C-80063
6-Chloro-4-hexen-1-ol, C-80064
6-Chloro-5-hexen-3-ol, C-80065
3-Chloro-4-hydroxybenzaldehyde, C-60089
4-Chloro-3-hydroxybenzaldehyde, C-60090
3-Chloro-4-hydroxybenzoic acid, C-60091
3-Chloro-5-hydroxybenzoic acid, C-60092
4-Chloro-3-hydroxybenzoic acid, C-60093
2-Chloro-3-hydroxy-7-chamigren-9-one, C-60094
3-Chloro-4-hydroxy-3-cyclobutene-1,2-dione, C-70071
2-Chloro-1-hydroxy-5,8-dimethoxy-6-methylxanthone, *in* T-70181
5-Chloro-8-hydroxy-1,4-dimethoxy-3-methylxanthone, *in* T-70181
10α-Chloro-1β-hydroxy-11(13)-eremophilen-12,8β-olide, *in* D-80314
β-Chloro-α-hydroxyethylbenzene, *see* C-80099
3-Chloro-6-hydroxy-2-methoxybenzaldehyde, *in* C-60058
5-Chloro-2-hydroxy-3-methoxybenzaldehyde, *in* C-70065
2-Chloro-3-hydroxy-5-methylbenzoic acid, C-60095
3-Chloro-4-hydroxy-5-methylbenzoic acid, C-60096
5-Chloro-4-hydroxy-2-methylbenzoic acid, C-60097
3-Chloro-5-hydroxy-2-methyl-1,4-naphthalenedione, *see* C-60098
3-Chloro-5-hydroxy-2-methyl-1,4-naphthoquinone, C-60098
2-Chloro-5-hydroxy-6-methylpyridine, C-60099
2-Chloro-6-hydroxy-1,4-naphthalenedione, *see* C-80066
2-Chloro-7-hydroxy-1,4-naphthalenedione, *see* C-80067
2-Chloro-6-hydroxy-1,4-naphthoquinone, C-80066
2-Chloro-7-hydroxy-1,4-naphthoquinone, C-80067
6-Chloro-3-hydroxy-2-picoline, *see* C-60099
▷ 3-Chloro-2-hydroxypropanoic acid, C-70072
▷ 2-Chloro-3-hydroxypyridine, C-60100
2-Chloro-5-hydroxypyridine, C-60101
3-Chloro-5-hydroxypyridine, C-60102
4-Chloro-6-hydroxy-2(1*H*)-pyridinone, C-70073
6-Chloro-4-hydroxy-2(1*H*)pyridinone, C-70074
▷ 5-Chloro-8-hydroxyquinoline, C-70075
8-Chloro-9-hydroxy-1,5,5,9-tetramethylspiro[5.5]undec-1-en-3-one, *see* C-60094
5-Chloro-4-hydroxy-*m*-toluic acid, *see* C-60096
6-Chloro-5-hydroxy-*m*-toluic acid, *see* C-60095
5-Chloro-4-hydroxy-*o*-toluic acid, *see* C-60097
2-Chloro-1*H*-imidazole, C-70076
4(5)-Chloro-1*H*-imidazole, C-70077
2-Chloro-4,5-imidazolidinedione, *see* C-60054
2-Chloro-2-imidazoline, *see* C-80050
4-Chloro-1*H*-imidazo[4,5-*c*]pyridine, C-60104
6-Chloro-1*H*-imidazo[4,5-*c*]pyridine, C-60105
4-Chloroindoline, *see* C-60055
2-Chloroinosine, *see* C-70161
1-Chloro-1-iodoethane, C-60106
1-Chloro-2-iodoethane, C-70078
Chloroiodomethane, C-80068
2-Chloro-3-iodopyridine, C-60107
2-Chloro-4-iodopyridine, C-60108
2-Chloro-5-iodopyridine, C-60109
3-Chloro-2-iodopyridine, C-60110
3-Chloro-5-iodopyridine, C-60111
4-Chloro-2-iodopyridine, C-60112
4-Chloro-3-iodopyridine, C-60113
4-Chloro-1(3*H*)-isobenzofuranone, C-70079
7-Chloro-1(3*H*)-isobenzofuranone, C-70080
▷ 1-Chloro-2-isocyanatoethane, C-80069
▷ 1-Chloro-2-isothiocyanoethane, C-70081
β-Chlorolactic acid, *see* C-70072
Chloromaleic acid, *in* C-80043
2-Chloro-6-mercaptobenzoic acid, C-70082
3-Chloro-2-mercaptobenzoic acid, C-70083
4-Chloro-2-mercaptobenzoic acid, C-70084
5-Chloro-2-mercaptobenzoic acid, C-70085
3-Chloro-2-mercaptopyridine, *see* C-60129
Chloromethanesulfonic acid, C-70086
Chloromethanesulfonyl bromide, *in* C-70086
▷ Chloromethanesulfonyl chloride, *in* C-70086
Chloromethanol, C-80070
3-Chloro-4-methoxybenzaldehyde, *in* C-60089
4-Chloro-3-methoxybenzaldehyde, *in* C-60090
3-Chloro-4-methoxybenzoic acid, *in* C-60091
3-Chloro-5-methoxybenzoic acid, *in* C-60092
4-Chloro-3-methoxybenzoic acid, *in* C-60093
1-Chloro-4-methoxybenzo[*g*]phthalazine, *in* C-70055
2-Chloro-3-methoxy-2-cyclohexen-1-one, *in* C-80046
3-Chloro-3-methoxy-3*H*-diazirine, C-70087
2-(Chloromethoxy)ethanol acetate, *see* C-70088
2-(Chloromethoxy)ethyl acetate, C-70088
3-Chloro-2-(methoxymethoxy)-1-propene, C-70089
2-Chloro-3-methoxy-5-methylbenzoic acid, *in* C-60095
3-Chloro-4-methoxy-5-methylbenzoic acid, *in* C-60096
5-Chloro-4-methoxy-2-methylbenzoic acid, *in* C-60097
1-Chloro-5-methoxy-2-methyl-3-nitrobenzene, *in* C-60116
2-Chloro-1-methoxy-3-methyl-4-nitrobenzene, *in* C-60115
2-(Chloromethoxy)-2-methylpropane, *see* B-70295
4-Chloro-6-methoxy-1-methyl-2(1*H*)-pyridinone, *in* C-70073
4-Chloro-2-methoxy-1-nitrobenzene, *in* C-60119
2-Chloro-3-methoxy-6-nitrotoluene, *in* C-60115
2-Chloro-4-methoxy-6-nitrotoluene, *in* C-60116
2-Chloro-3-methoxypyridine, *in* C-60100
3-Chloro-5-methoxypyridine, *in* C-60102
6-Chloro-4-methoxy-2(1*H*)-pyridinone, *in* C-70074
α-(Chloromethyl)benzenemethanol, *see* C-80099
N-Chloro-4-methylbenzenesulfonamide, C-80071
1-Chloromethylbenz[*cd*]indol-2(1*H*)-one, *in* B-70027
α-Chloromethylbenzyl alcohol, *see* C-80099
Chloromethyl *tert*-butyl ether, *see* B-70295
2-Chloro-3-methyl-2-cyclopenten-1-one, C-70090
5-Chloro-3-methyl-2-cyclopenten-1-one, C-70091
2-(Chloromethyl)-3,5-dioxa-1-hexene, *see* C-70089
4-Chloro-5-methylfurazan, C-60114

3-Chloro-4-methylfuroxan, *in* C-60114
4-Chloro-3-methylfuroxan, *in* C-60114
1-(Chloromethyl)-1*H*-indole-2,3-dione, C-70092
N-Chloromethylisatin, *see* C-70092
1-(Chloromethyl)-2-methoxybenzene, *in* C-70101
1-(Chloromethyl)-3-methoxybenzene, *in* C-70102
1-Chloromethyl-4-methoxybenzene, *in* C-70103
2-(Chloromethyl)-3-methylpyridine, C-70093
▷ 2-(Chloromethyl)-4-methylpyridine, C-70094
2-(Chloromethyl)-5-methylpyridine, C-70095
▷ 2-(Chloromethyl)-6-methylpyridine, C-70096
3-(Chloromethyl)-2-methylpyridine, C-70097
3-(Chloromethyl)-4-methylpyridine, C-70098
▷ 4-(Chloromethyl)-2-methylpyridine, C-70099
5-(Chloromethyl)-2-methylpyridine, C-70100
2-Chloro-3-methyl-4-nitroanisole, *in* C-60115
2-Chloro-3-methyl-4-nitrophenol, C-60115
3-Chloro-4-methyl-5-nitrophenol, C-60116
4-Chloro-5-methyl-1,2,5-oxadiazole, *see* C-60114
▷ (Chloromethyl)pentafluorobenzene, C-80072
5-Chloro-3-methyl-1-pentene, C-60117
1-(Chloromethyl)phenanthrene, C-80073
2-(Chloromethyl)phenanthrene, C-80074
3-(Chloromethyl)phenanthrene, C-80075
4-(Chloromethyl)phenanthrene, C-80076
9-(Chloromethyl)phenanthrene, C-80077
2-(Chloromethyl)phenol, C-70101
3-(Chloromethyl)phenol, C-70102
4-(Chloromethyl)phenol, C-70103
Chloromethylphenylcarbinol, *see* C-80099
1-Chloro-4-methylphthalazine, C-70104
2-Chloro-3-methylpyrazine, C-70105
2-Chloro-5-methylpyrazine, C-70106
2-Chloro-6-methylpyrazine, C-70107
3-Chloro-2-methylpyrazine 1-oxide, *in* C-70105
3(5)-Chloro-5(3)-methylpyrazole, C-70109
▷ 4-Chloro-3(5)methylpyrazole, C-70108
3-Chloro-1-methylpyrazole, *in* C-70155
4-Chloro-1-methylpyrazole, *in* C-70156
5-Chloro-1-methylpyrazole, *in* C-70155
3-Chloro-4-methylpyridazine, C-70110
3-Chloro-5-methylpyridazine, C-70111
3-Chloro-6-methylpyridazine, C-70112
4-Chloro-3-methylpyridazine, C-80078
4-Chloro-5-methylpyridazine, C-80079
6-Chloro-2-methyl-3-pyridinol, *see* C-60099
2-Chloro-4-methylpyrimidine, C-70113
2-Chloro-5-methylpyrimidine, C-70114
4-Chloro-2-methylpyrimidine, C-70115
4-Chloro-5-methylpyrimidine, C-70116
4-Chloro-6-methylpyrimidine, C-70117
5-Chloro-2-methylpyrimidine, C-70118
5-Chloro-4-methylpyrimidine, C-70119
2-Chloro-3-methylquinoxaline, C-70121
2-Chloro-5-methylquinoxaline, C-70122
2-Chloro-6-methylquinoxaline, C-70123
2-Chloro-7-methylquinoxaline, C-70124
2-(Chloromethyl)quinoxaline, C-70120
6-Chloro-7-methylquinoxaline, C-70125
3-Chloro-7-methylquinoxaline 1-oxide, *in* C-70123
3-Chloro-2-(methylsulfonyl)pyridine, *in* C-60129
5-Chloro-2-(methylthio)benzoic acid, *in* C-70085
2-Chloro-6-(methylthio)benzonitrile, *in* C-70082
3-Chloro-2-(methylthio)pyridine, *in* C-60129
2-Chloro-1-naphthalenamine, *see* C-80080
6-Chloro-1,2,3,4-naphthalenetetrol, C-60118
2-Chloro-1-naphthylamine, C-80080
3-Chloro-3-(1-naphthylmethyl)diazirine, C-80081
2-Chloronebularine, *see* C-70159
6-Chloronebularine, *see* C-70160
1′-Chloronephroarctin, *in* N-70032
4′-Chloronephroarctin, *in* N-70032
2-Chloro-2-nitroadamantane, C-80082
5-Chloro-2-nitroanisole, *in* C-60119
2-Chloro-6-nitrobenzenemethanamine, *see* C-70126
4-Chloro-2-nitrobenzenemethanamine, *see* C-70127
4-Chloro-3-nitrobenzenemethanamine, *see* C-70128
5-Chloro-2-nitrobenzenemethanamine, *see* C-70129
2-Chloro-6-nitrobenzylamine, C-70126
4-Chloro-2-nitrobenzylamine, C-70127
4-Chloro-3-nitrobenzylamine, C-70128
5-Chloro-2-nitrobenzylamine, C-70129
2-Chloro-4-nitro-*m*-cresol, *see* C-60115
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1-Chloro-1-nitrocyclohexane, C-70131
2-Chloro-3-nitro-9*H*-fluorene, C-70132
2-Chloro-7-nitro-9*H*-fluorene, C-70133
9-Chloro-2-nitro-9*H*-fluorene, C-70134
9-Chloro-3-nitro-9*H*-fluorene, C-70135
5-Chloro-2-nitrophenetole, *in* C-60119
▷ 5-Chloro-2-nitrophenol, C-60119
▷ 2-Chloro-2-nitropropane, C-60120
1-Chloro-2-nitrosobenzene, C-80083
1-Chloro-3-nitrosobenzene, C-80084
1-Chloro-4-nitrosobenzene, C-80085
2-Chloro-2-nitrotricyclo[3.3.1.1^{3,7}]decane, *see* C-80082
4-Chloro-1-nitro-2-(trifluoromethyl)benzene, C-80086
2-Chloronorbornadiene, *see* C-70056
5-Chloro-2-(2,4,6-octatriynylidene)-3,7-dioxabicyclo[4.1.0]heptane, *in* C-80051
5-Chloroorsellinaldehyde, *see* C-60060
Chloropanaxydiol, *in* P-80006
5-Chloro-1,3-pentadiene, C-60121
2-Chloro-4-[5-(1,3-pentadiynyl)-2-thienyl]-3-butyn-1-ol, *in* P-80025
1-Chloro-2,3,3,4,4-pentafluorocyclobutene, C-80087
1-Chloro-1,1,3,3,3-pentafluoropropane, C-80088
1-Chloro-2,2,3,3,3-pentafluoropropane, C-80089
1-Chloro-1,2,3,3,3-pentafluoro-1-propene, C-80090
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4-Chloro-4-penten-1-ol, C-80091
5-Chloro-1-pentyne, C-70139
2-Chloro-1*H*-perimidine, C-80092
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2-Chloro-1-phenazinecarboxylic acid, C-80093
3-Chloro-1-phenazinecarboxylic acid, C-80094
6-Chloro-1-phenazinecarboxylic acid, C-80095
7-Chloro-1-phenazinecarboxylic acid, C-80096
8-Chloro-1-phenazinecarboxylic acid, C-80097
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4-Chlorophenylphenylmethanol, *see* C-60065
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1-(2-Chloro-3-pyridinyl)ethanone, *see* A-70034
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CP 54883, *see* A-70222
Crassifolioside, C-80155
Crataegin, *in* D-84287
Cratystyolide, *in* T-70257
Crepidatin, *in* D-80371
Crepiside *A*, *in* Z-60001
Crepiside *B*, *in* Z-60001
m-Cresol-4-aldehyde, *see* H-70161
m-Cresol-5-aldehyde, *see* H-80195
m-Cresol-6-aldehyde, *see* H-70160
m-Cresol-4-carboxylic acid, *see* H-70164
m-Cresol-6-carboxylic acid, *see* H-70163
2,4-Cresotaldehyde, *see* H-70160
3,5-Cresotaldehyde, *see* H-80195
4,2-Cresotaldehyde, *see* H-70161
2,4-Cresotic acid, *see* H-70163
4,2-Cresotic acid, *see* H-70164
Cristacarpin, C-80156
Croconate blue, *in* T-70321
Crombeone, C-70200
Crotalarin, C-60171
Crotarin, C-60172
Crotmadine, C-80157
Crotonin, C-80158
t-Crotonin, *in* C-80158
2-Crotonyloxymethyl-4,5,6-trihydroxy-2-cyclohexenone, *see* T-60338
▷ Crotylamine, *see* B-80278
Croweacic acid, *in* H-60177
12-Crown-3, *see* T-70304
Crustaxanthin, C-80159
Crustecdysone, *in* H-60063
Cryptand 2.2.1, *see* P-60060
▷ Cryptand 222, *see* H-60073
Cryptanol, *see* A-60006
Cryptolepine, *in* I-70016
Cryptomerin *A*, *in* H-60082
Cryptomerin *B*, *in* H-60082
Cryptopimaric acid, *see* S-80008
Cryptoresinol, C-70201
Cryptotanshinone, C-60173
Crystal violet lactone, C-70202
CS 280, *see* S-60029
Cubanecarboxylic acid, C-60174
Cubene, C-80160
Cucurbic acid, C-50302
▷ Cucurbitacin *D*, C-70203
▷ Cucurbitacin *E*, C-70204
▷ Cucurbitacin *I*, *in* C-70204
Cucurbitacin *L*, *in* C-70204
Cucurbitacin *R*, *in* C-70203
Cucurbitacin T, C-80162
5,24-Cucurbitadiene-3,11,26-triol, C-60175
Cudraflavone *A*, C-70205
Cudraisoflavone *A*, C-70206
Cudraniaxanthone, C-80163
Cumambranolide, C-80164
Cumambrin A, *in* C-80164
Cumambrin B, *in* C-80164
▷ *p*-Cumaric acid, *see* H-80242
▷ Cumic alcohol, *see* I-80078
▷ Cuminyl alcohol, *see* I-80078
Cumotocopherol, *see* T-80200
Cuneatin, *in* T-80107
Cuneatin methyl ether, *in* T-80107
▷ Cupferron, *in* H-70208
Curcudiol, C-70207
Curculathyrane *A*, C-60176
Curculathyrane *B*, C-60177
Curcuma yellow, *see* C-80165
Curcumin, C-80165
Curcumone, *see* M-60112
Curcuphenol, C-70208
Curramycin *B*, *in* C-60178
Curromycin *A*, C-60178
Curvularin, C-80166
▷ Cyanic acid, C-80167
1-Cyanoacenaphthene, *in* A-70014
o-Cyanoacetophenone, *in* A-80015
9-Cyanoacridine, *in* A-70061
2-Cyanobenzanthrone, *in* O-80059
3-Cyanobenzanthrone, *in* O-80060
4-Cyanobenzanthrone, *in* O-80061
N-Cyanobenzenecarboximidoyl chloride, C-80168
2-Cyano-1,4-benzodioxan, *in* B-60024
o-Cyanobenzophenone, *in* B-80054
1-Cyano-2-benzoyl-1,2-dihydroisoquinoline, *see* B-70073
1-Cyanobicyclo[1.1.0]butane, *in* B-70094
2-Cyanobicyclo[2.2.1]hepta-2,5-diene, *in* B-60084
1-Cyanobiphenylene, *in* B-80109
2-Cyanobiphenylene, *in* B-80110
4-Cyanobutanal, *in* O-80089
1-Cyanochrysene, *in* C-80128
3-Cyanochrysene, *in* C-80130
5-Cyanochrysene, *in* C-80131
6-Cyanochrysene, *in* C-80132
1-Cyanocycloheptene, *in* C-80178
4-Cyanocyclohexanethiol, *in* M-60020
Cyanocyclooctatetraene, *in* C-70239
2-Cyanocyclopentanone, *in* O-70084
1-Cyanocyclopropanecarboxylic acid, *in* C-80196
5-Cyano-7-deazaguanosine, *see* A-70132
2-Cyano-1,2-dihydrocyclobuta[*a*]naphthalene, *in* D-70177
1-Cyano-4,5-dimethoxy-2-nitrobenzene, *in* D-60360
4-Cyano-2,2-dimethylbutyraldehyde, *in* D-60434
2-Cyano-1,1-dimethylcyclopropane, *in* D-80444
5-Cyano-3,3-dimethyl-1-nitro-1-pentene, *in* D-60429
4-Cyano-2,5-dimethyloxazole, *in* D-80461
▷ 1-Cyano-3,5-dinitrobenzene, *in* D-60458
2-Cyano-1,3-dinitrobenzene, *in* D-60457
1-Cyano-1,1-diphenylethane, *in* D-70493
Cyanododecahedrane, *in* D-80522
2-Cyanoethanethioamide, C-70209
▷ Cyanoethylene, *in* P-70121
▷ *N*-(2-Cyanoethyl)glycine, *in* C-60016
2-Cyano-3-fluoroaniline, *in* A-70143
3-Cyano-4-fluoroaniline, *in* A-70147
4-Cyano-2-fluoroaniline, *in* A-70146
4-Cyano-3-fluorobenzenethiol, *in* F-70029
2-Cyano-1-fluoro-3-iodobenzene, *in* F-70020
2-Cyanofuro[2,3-*b*]pyridine, *in* F-60098
2-Cyanofuro[3,2-*b*]pyridine, *in* F-60100
3-Cyanofuro[2,3-*b*]pyridine, *in* F-60099
3-Cyanofuro[3,2-*b*]pyridine, *in* F-60101
2-Cyanofuro[2,3-*c*]pyridine, *in* F-60102
2-Cyanofuro[3,2-*c*]pyridine, *in* F-60104
3-Cyanofuro[2,3-*c*]pyridine, *in* F-60103
3-Cyanofuro[3,2-*c*]pyridine, *in* F-60105
▷ Cyanogen fluoride, C-80169
1-Cyano-3-hexyne, *in* H-80032
6-Cyano-1-hexyne, *in* H-80033
3-Cyano-2-hydroxy-5-nitrobenzoic acid, *in* H-70188
2-Cyano-3-hydroxyquinoline, *in* H-60228
3-Cyano-2-hydroxy-*N*,*N*,*N*-trimethylpropanaminium, *in* C-70024
4(5)-Cyanoimidazole, *in* I-60004
3-Cyanoindole, *in* I-80012
2-Cyano-3-iodothiophene, *in* I-60075
2-Cyano-4-iodothiophene, *in* I-60076
2-Cyano-5-iodothiophene, *in* I-60078
3-Cyano-2-iodothiophene, *in* I-60074
3-Cyano-4-iodothiophene, *in* I-60077
4-Cyano-2-iodothiophene, *in* I-60079
5-Cyanoisoxazole, *in* I-60142
1-Cyano-3-methylbicyclo[1.1.0]butane, *in* M-70053
4-(Cyanomethyl)coumarin, *in* O-60057
Cyano methyl disulfide, *see* M-60032
▷ 3-Cyanomethyl-1*H*-indole, *in* I-70013
(Cyanomethyl)pentafluorobenzene, *in* P-80027
1-(Cyanomethyl)phenanthrene, *in* P-70046
9-Cyanomethylphenanthrene, *in* P-70047
3-Cyano-10-methylphenothiazine, *in* P-70057
2-Cyano-1-methyl-4-phenyl-1-thianaphthalene, *see* M-80142
3-Cyano-2-methyl-2-propenoic acid, *in* M-70103
1-Cyano-2-methyl-1-propen-1-ol, *see* H-80198
N-(4-Cyano-1-methyl-1*H*-pyrazol-5-yl)acetamide, *in* A-70192
3-Cyano-2-naphthoic acid, *in* N-80001
6-Cyano-2-pentene, *in* H-70024
5-Cyano-1-pentyne, *in* H-80086
2-Cyanophenol, *in* H-70108
2-Cyano-10*H*-phenothiazine, *in* P-70056
▷ 3-Cyano-10*H*-phenothiazine, *in* P-70057
Cyano phenyl disulfide, *see* B-60013
4-Cyano-2-phenyl-1,2,3-triazole, *in* P-60140
3-Cyanopropanal, *in* O-80068
▷ 1-Cyano-2-propen-1-ol, *in* P-70119
1-Cyano-2,3,4,5-tetrafluorobenzene, *in* T-70032
3-Cyano-1,2,4,5-tetrafluorobenzene, *in* T-70034
2-Cyanotetrahydrothiophene, *in* T-70099
2-Cyanothioacetamide, *see* C-70209
4-Cyano-1,2,3-triazole, *in* T-60239
1-Cyano-2,4,5-trifluorobenzene, *in* T-70240
▷ 2-Cyano-3,3,3-trifluoropropene, *in* T-60295
1-Cyano-2,3,5-trimethoxybenzene, *in* T-70250
2-Cyanotriphenylene, *in* T-60384

Cyanoviridin *RR*, C-70210
▷ Cyanuric acid, C-60179
▷ Cyclic (L-asparaginyl-4-hydroxy-L-prolyl-(*R*)-4,5-dihydroxy-L-isoleucyl-6-hydroxy-2-mercapto-L-tryptophylglycyl-L-isoleucylglycyl-L-cysteinyl) cyclic(4→8)-sulfide (*R*)-*S*-oxide, *in* A-60084
Cyclic(*N*-methyl-L-alanyl-L-tyrosyl-D-tryptophyl-L-lysyl-L-valyl-L-phenylalanyl), C-60180
Cyclo(alanylaspartyl), *see* M-60064
Cycloanticopalic acid, C-60181
Cycloaraneosene, C-80170
3,16,24,25,30-Cycloartanepentol, C-60182
23-Cycloartene-3,25-diol, C-80171
24-Cycloartene-1,3-diol, C-80172
Cycloartobiloxanthone, C-80173
Cycloaspeptide *A*, C-70211
Cycloaspeptide *B*, *in* C-70211
Cycloaspeptide *C*, *in* C-70211
Cyclobuta[*b*]anthracen-1(2*H*)one, C-80174
▷ 4,5-Cyclobuta-1,2-benzoquinone, *see* B-70110
1,3-Cyclobutadiene, C-70212
Cyclobuta[*b*]naphthalen-1(2*H*)-one, C-80175
1,1-Cyclobutanedimethanethiol, C-70213
1,2-Cyclobutanedimethanethiol, C-70214
1,2-Cyclobutanedione, C-60183
1,1-Cyclobutanedithiol, C-70215
1,3-Cyclobutanedithiol, C-60184
1,1′-(1,2-Cyclobutanediylidenedimethylidyne) bisbenzene, *see* D-60083
1,1′,1″,1‴-(1,2,3,4-Cyclobutanetetraylidene) tetrakiscyclohexane, *see* T-80130
Cyclobutylidenecyclobutane, *see* B-70095
(Cyclobutylidenemethyl)benzene, *see* B-70081
Cyclobutylidenephenylmethane, *see* B-70081
Cyclocaducinol, C-80176
24,26-Cyclo-5,22-cholestadien-3β-ol, *see* P-60004
(24*S*,25*S*)-24,26-Cyclo-5α-cholest-22*E*-en-3β-ol, *in* P-60004
Cyclocratystyolide, C-70216
2,7-Cyclodecadien-1-one, C-60185
3,7-Cyclodecadien-1-one, C-60186
Cyclodeca[1,2,3-*de*:6,7,8-*d′e′*]dinaphthalene, C-60187
Cyclo[*d.e.d.e.e.d.e.d.e.e*]decakisbenzene, *see* D-60396
3-Cyclodecene-1,5-diyne, C-80177
Cyclodehydromyopyrone *A*, C-60188
Cyclodehydromyopyrone *B*, C-60189
1,4,7,10-Cyclododecatetraene, C-70217
1,5,9-Cyclododecatrien-3-yne, C-60190
1-Cyclododecenecarboxaldehyde, C-60191
Cyclododecyne, C-60192
Cycloeuphordenol, C-70218
Cyclofoetigenin *B*, *in* C-60182
β-Cyclohallerin, *in* C-60193
α-Cyclohallerin, C-60193
Cyclohepta[1,2-*b*:1,7-*b′*]bis[1,4]benzoxazine, C-70219
Cyclohepta[*def*]carbazole, C-70220
Cyclohepta[*def*]carbazolium tetrafluoroborate, *in* C-70220
Cyclohept[*fg*]acenaphthylene-5,6-dione, C-60194
Cyclohept[*fg*]acenaphthylene-5,8-dione, C-60195
2,6-Cycloheptadien-4-yn-1-one, C-60196
Cyclohepta[*ef*]heptalene, C-60197
Cyclohepta[*de*]naphthalene, C-60198
peri-Cycloheptanaphthalene, *see* C-60198
Cyclohepta[*a*]phenalene, C-60199
5*H*-Cyclohepta[4,5]pyrrolo[2,3-*b*]indole, C-60200
Cyclohepta[*b*]pyrrol-2(1*H*)-one, C-60201
1,3,5-Cycloheptatriene-1,6-dicarboxylic acid, C-60202
2,4,6-Cycloheptatriene-1-thione, C-60203
2,4,6-Cycloheptatrien-1-one, C-60204
3-(1,3,6-Cycloheptatrien-1-yl-2,4,6-cycloheptatrien-1-ylidenemethyl)-1,3,5-cycloheptatriene, C-60205
2,4,6-Cycloheptatrienyl cyclopropyl ketone, *see* C-60206
2,4,6-Cycloheptatrien-1-ylcyclopropylmethanone, C-60206
4-(2,4,6-Cycloheptatrien-1-ylidene)bicyclo[5.4.1]dodeca-2,5,7,9,11-pentaene, C-60207
5-(2,4,6-Cycloheptatrien-1-ylidene)-3,6-cycloheptadiene-1,2-dione, *see* H-60022
2-(2,4,6-Cycloheptatrien-1-ylidene)-1,3-dithiane, C-70221
5-(2,4,6-Cycloheptatrien-1-ylideneethylidene)-3,6-cycloheptadiene-1,2-dione, C-70222
Cycloheptatrienylidene(tetraphenylcyclopentadenylidene)ethylene, C-60208
1-Cycloheptenecarboxylic acid, C-80178
2-Cycloheptene-1,4-diol, C-80179
2,3-Cycloheptenonaphthalene, *see* T-70047
1-(1-Cyclohepten-1-yl)ethanone, *see* A-60026
▷ 2,5-Cyclohexadiene-1,4-dione, *see* B-70044
1,1′,1″,1‴-(2,5-Cyclohexadiene-1,4-diylidenedimethanetetrayl)tetrakisbenzene, *see* B-60157
1,3-Cyclohexadien-5-yne, *see* B-70087
1*H*-Cyclohexa[4,5,6-*de*]methano[10]annulen-1-one, *see* M-70042
1,1-Cyclohexanedimethanethiol, C-70223
1,2-Cyclohexanedimethanethiol, C-70224
▷ 1,1-Cyclohexanedithiol, C-60209
1,2-Cyclohexanedithiol, C-70225
(1α,2α,3α,4β,5α,6β)-Cyclohexanehexol, *see* I-80015
Cyclohexanehexone, C-60210
1,3,5-Cyclohexanetricarboxaldehyde, C-70226
Cyclohexanol-2-carboxylic acid, *see* H-70119
Cyclohexanone isoxime, *see* O-70052
Cyclohexano[*b*]-2-oxazolidone, *see* H-70052
3-Cyclohexene-1-carboxaldehyde, C-70227
4-Cyclohexene-1,2-diamine, C-80180
4-Cyclohexene-1,2-dicarboximide, *see* T-80070
2-Cyclohexene-1,4-diol, C-80181
4-Cyclohexene-1,2-diol, C-80182
1,2-Cyclohexenoacenaphthylene, *see* T-70061
3-Cyclohexen-1-one, C-60211
9,10-Cyclohexenophenanthrene, *see* T-80082
Cyclohexeno-1,2,3-thiadiazole, *see* T-70042
1-(1-Cyclohexen-1-yl)ethanone, *see* A-70038
3-Cyclohexenyl methyl ketone, *see* A-70039
2-(1-Cyclohexenyl)propanal, C-80183
α-Cyclohexylcyclohexanemethanol, *see* D-70150
1-Cyclohexylcyclohexene, *see* D-60009
3-Cyclohexylcyclohexene, *see* D-60008
4-Cyclohexylcyclohexene, *see* D-60007
Cyclohexylglycollic acid, *see* C-60212
2-Cyclohexyl-2-hydroxyacetic acid, C-60212
α-Cyclohexyl-α-hydroxybenzeneacetic acid(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)methyl ester, *see* O-60102
▷ *N*-Cyclohexylhydroxylamine, C-70228
1,2-*O*-Cyclohexylidene-*myo*-inositol, *in* I-80015
2-Cyclohexyl-2-methoxyacetic acid, *in* C-60212
▷ Cyclohexyl phenyl ketone, *see* B-70071
▷ Cyclohexylphenylmethanone, *see* B-70071
2-Cyclohexylpropanal, C-80184
Cyclo(hydroxyprolylhydroxyprolyl), *see* O-60013
Cyclo(hydroxyprolylleucyl), C-60213
Cyclo(hydroxyprolylprolyl), *see* O-60017
3,12-Cycloiceane, *see* P-70019
Cyclo(isoleucylisoleucyl), *see* B-70153
9,19-Cyclolanost-23-ene-3,25-diol, *see* C-80171
Cyclo(leucylalanyl), *see* M-70118
Cyclo(leucylleucyl), *see* B-60171
Cyclo(leucylprolyl), C-80185
Cyclolongipesin, C-60214
Cyclolycoserone, C-70229
3*H*-Cyclonona[*def*]biphenylene, C-60215
3*H*-Cyclonona[*def*]biphenylen-3-one, C-70230
Cyclonona[*c*]furan, *see* H-60047
Cycloocta[*def*]biphenylene-1,4-dione, C-80186
1,5-Cyclooctadiene monoxide, *see* O-70058
Cycloocta[1,2-*b*:5,6-*b′*]dinaphthalene, C-60216
Cycloocta[2,1-*b*:3,4-*b′*]di[1,8]naphthyridine, C-70231
Cycloocta[2,1-*b*:3,4-*b′*]diquinoline, C-70232
Cycloocta[*def*]fluorene, C-70233
Cycloocta[*a*]naphthalene, C-70234
Cycloocta[*b*]naphthalene, C-70235
Cycloocta[*def*]phenanthrene, C-80187
1*H*-Cyclooctapyrazole, C-70236
1,3,5,7-Cyclooctatetraene-1-acetic acid, C-70237
Cyclooctatetraenecarboxaldehyde, C-70238
Cyclooctatetraenecarboxylic acid, C-70239
1,3,5-Cyclooctatriene, C-80188
1,3,5-Cyclooctatrien-7-yne, C-70240
1-Cyclooctene-1-acetic acid, C-70241
4-Cyclooctene-1-acetic acid, C-70242
1-Cyclooctenecarboxaldehyde, C-60217
1-(1-Cyclooctenyl)ethanone, *see* A-60027
(1-Cyclooctenyl) methyl ketone, *see* A-60027
Cycloorbicoside *A*, *in* C-60218
Cycloorbigenin, C-60218
▷ Cyclopentadecanone, C-60219
Cyclopentadecyne, C-60220
1,1′,1″,1‴-(1,3-Cyclopentadiene-1,2,3,4-tetrayl)tetrakisbenzene, *see* T-70149
5-(2,4-Cyclopentadien-1-ylidene)-1,3-cyclopentadiene, *see* F-60080
2-(2,4-Cyclopentadien-1-ylidene)-1,3-dithiolane, *in* C-60221
2-(2,4-Cyclopentadienylidene)-1,3-dithiole, C-60221
5*H*-Cyclopenta[2,1-*c*:3,4-*c′*]dipyridin-5-one, *see* D-70053
1,1-Cyclopentanedimethanethiol, C-70243
1,2-Cyclopentanediol, C-80189
1,1-Cyclopentanedithiol, C-60222
Cyclopentanone-2-carboxylic acid, *see* O-70084
▷ 4*H*-Cyclopenta[*def*]phenanthrene, C-70244
1*H*-Cyclopenta[*l*]phenanthrene, C-80190
Cyclopenta[*cd*]pleiadene, C-80191
Cyclopenta[*c*]pyran, C-80192
▷ Cyclopenta[*cd*]pyrene, C-60223
Cyclopenta[*b*]thiapyran, C-60224
Cyclopenta[*b*]thiophene, *see* D-70180
Cyclopenta[*c*]thiophene, *see* D-70181
4*H*-Cyclopenta[*c*]thiophen-5(6*H*)-one, C-70245
Cyclopent[*b*]azepine, C-60225
4-Cyclopentene-1,3-diol, C-80193
3-Cyclopentene-1-glyoxal, *see* O-60061
2,3-Cyclopentenonaphthalene, *see* B-60015
2-Cyclopenten-1-one, C-60226
9,10-Cyclopentenophenanthrene, *see* D-80177
2,3-Cyclopentenopyridine, *see* D-60275
3,4-Cyclopentenopyridine, *see* D-60276
Cyclopenteno-1,2,3-thiadiazole, *see* D-70179
1-(1-Cyclopenten-1-yl)ethanone, *see* A-60028
1-Cyclopenten-1-ylmethyl ketone, *see* A-60028
1-Cyclopentenyl phenyl ketone, *see* B-70072
1-Cyclopenten-1-ylphenylmethanone, *see* B-70072
2-Cyclopentylidenecyclopentanone, C-60227
(Cyclopentylidenemethyl)benzene, *see* B-70083
Cyclopentylidenephenylmethane, *see* B-70083
Cyclopentyl phenyl ketone, *see* B-80055
Cyclopentylphenylmethanone, *see* B-80055
2-Cyclopentylpropane, *see* I-70092
[2.2.2](1,2,3)Cyclophane, C-60228
[2.2.2](1,2,3)Cyclophane-1,9-diene, C-60229
$13^2,17^3$-Cyclopheophorbide enol, C-60230
Cyclo(prolylalanyl), C-80194
Cyclo(prolylisoleucyl), *see* H-60052
Cyclo(prolylprolyl), *see* O-60016
1*H*-Cyclopropabenzene, C-70246
Cyclopropa-*p*-benzoquinone, *see* B-80078
5*H*-Cyclopropa[*f*][2]benzothiophene, C-70247
Cyclopropadodecahedrane, C-80195
1,1-Cyclopropanedicarboxylic acid, C-80196
1,2-Cyclopropanedicarboxylic acid, C-70248

1,1-Cyclopropanedimethanethiol, C-70249
Cyclopropaneglyoxylic acid, *see* C-60231
Cyclopropanehexacarboxylic acid, C-70250
9,9′,9″-(1,2,3-Cyclopropanetriylidene)tris-9*H*-fluorene, *see* T-70322
9,9′,9″-(1,2,3-Cyclopropanetriylidene)tris-9*H*-thioxanthene, *see* T-70326
1*H*-Cyclopropa[*l*]phenanthrene, C-80197
5*H*-Cyclopropa[*f*]isobenzofuran, C-70251
Cyclopropylacetylene, *see* E-70045
4-Cyclopropyl-1-buten-3-yne, *see* B-70293
1,1′-Cyclopropylidenebisbenzene, *see* D-60478
1,1′-Cyclopropylidenebisethanone, *see* D-70032
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2′-Deoxyinosine, D-70023
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2′-Deoxymugeneic acid, *in* M-60148
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3′,4′-Deoxypsorospermin-3′,4′-diol, *in* D-60021
5-Deoxypulchelloside *I*, *in* P-70139
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15-Desacetyltetraneurin *C* isobutyrate, *in* T-60158
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Desoxodehydrolaserpitin, *in* D-70009
Desoxyarticulin, *in* A-60307
5-Desoxyeuparotin, *in* E-80090
3-Desoxyjuslimtetrol, *see* R-60012
6-Desoxyleucotylin, *in* H-80096
8-Desoxyurospermal A, *in* I-80102
Dess-Martin periodinane, *see* T-60228
Des-A-26,27,28-trisnorursa-5,7,9,11,13,15,17-heptaene, D-80038
Des-A-5(10),12-ursadiene, D-80039
Detoxinine, D-80040
Detrothyronine, *in* T-60350
Dewar furan, *see* O-70059
▷ Dexcyanidanol, *in* P-70026
Dextrosapinic acid, *in* A-80001
Dextrothyronine, *in* T-60350
1,10-Diaazaanthracene, *see* B-80030
1,9-Diaazaanthracene, *see* B-80032
1,3-Diacetin, *see* D-60023
1α,2α-Diacetoxyalantolactone, *in* I-80046
3α,20-Diacetoxy-2α-angeloyloxy-9α,13*R*-epoxy-7,14-labdadiene, *in* E-80035
3α,20-Diacetoxy-2α-angeloyloxy-8,14-labdadiene-7α,13*R*-diol, *in* L-80005
3α,20-Diacetoxy-2α-angeloyloxy-8(17),14-labdadiene-7α,13*R*-diol, *in* L-80006
12,13-Diacetoxy-1(10)-aromadendren-2-one, *in* D-70283
6β,9β-Diacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran, *in* T-80090
9α,14-Diacetoxy-1α-benzoyloxy-4β,6β,8β-trihydroxydihydro-β-agarofuran, *in* E-60018
ent-6β,17-Diacetoxy-14,15-bisnor-7,11*E*-labdadien-13-one, *in* D-60311
2α,16-Diacetoxy-15-bromo-9(11)-pargueren-7α-ol, *in* B-80240
3,14-Diacetoxy-2-butanoyloxy-5,8(17)-briaradien-18,7-olide, *in* E-70012
4,14-Diacetoxy-2-butanoyloxy-5,8(17)-briaradien-18,7-olide, *in* E-70012
5-(3,4-Diacetoxy-1-butynyl)-2,2′-bithienyl, *in* B-80166
5-(3,4-Diacetoxy-1-butynyl)-5′-methyl-2,2′-bithiophene, *in* M-70054
9α,14-Diacetoxy-1α,8β-dibenzoyloxy-4β,8β-dihydroxydihydro-β-agarofuran, *in* E-60018
3,4-Diacetoxy-3,4-dihydro-2,5(2*H*,5*H*)-furandione, *in* T-70005
ent-3α,6β-Diacetoxy-2α,11β-dihydroxy-16-kauren-15-one, *in* P-80047
ent-1β,3α-Diacetoxy-11α,15α-dihydroxy-16-kauren-6-one, *in* K-80008
3α,22-Diacetoxy-7α,15α-dihydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111
9β,20-Diacetoxy-2β,3α-dihydroxy-1(15),8(19)-trinervitadiene, *in* T-70296
1,2-Diacetoxy-5,6-dimethoxyphenanthrene, *in* T-60115
6,16-Diacetoxy-3,7-dolabelladien-12-ol, *in* D-70541
3β,30-Diacetoxyfriedelane, *in* F-80083
6α,11β-Diacetoxygedunin, *in* G-70006
9β,15-Diacetoxy-1(10),4,11(13)-germacratrien-12,6α-olide, *in* D-60324
3,7*a*-Diacetoxyhexahydro-2-oxa-3*a*,7-dimethyl-1,4-indanedione, *in* H-70055
8β,10β-Diacetoxyhirsutinolide 13-*O*-acetate, *in* H-80089
1β,6α-Diacetoxy-4α-hydroxy-11-eudesmen-12,8α-olide, *in* T-70259
3α,7α-Diacetoxy-15α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60327
3α,22ξ-Diacetoxy-15α-hydroxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318
3α,15α-Diacetoxy-22*R*-hydroxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318
3β,15α-Diacetoxy-22*R*-hydroxy-7,9(11)24-lanostatrien-26-oic acid, *in* T-80318
15α,22*S*-Diacetoxy-3α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
3α,22*S*-Diacetoxy-15α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
15α,22*S*-Diacetoxy-3β-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
3α,22-Diacetoxy-15α-hydroxy-7α-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111
2α,7α-Diacetoxy-6β-isovaleroyloxy-8,13*E*-labdadien-15-ol, *in* L-60002
ent-3β,17-Diacetoxy-16β-kauranol, *in* K-60005
ent-1β,3α-Diacetoxy-16-kaurene-6β,11α,15α-triol, *in* K-80008
ent-3β,19-Diacetoxy-15-kauren-17-oic acid, *in* D-60341
ent-6β,17-Diacetoxy-7,12*E*,14-labdatriene, *in* L-60004
ent-6β,17-Diacetoxy-7,11*E*,14-labdatrien-13ξ-ol, *in* L-60005
15,17-Diacetoxy-7-labdene, *in* L-80012
7β,15-Diacetoxy-8-labden-17-oic acid, *in* D-80330
3β,15α-Diacetoxy-8,24-lanostadien-26-oic acid, *in* D-80331
3α,15α-Diacetoxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314
3β,15α-Diacetoxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314
3β,23-Diacetoxy-20(30)-lupen-29-al, *in* D-70316
3α,22-Diacetoxy-7α-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60328
8β,10β-Diacetoxy-1-*O*-methylhirsutinolide 13-*O*-acetate, *in* H-80089
6α,17α-Diacetoxy-15,17-oxido-16-spongianone, *in* D-60365
3α,15α-Diacetoxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70330
4,14-Diacetoxy-2-propanoyloxy-5,8(17)-briaradien-18,7-olide, *in* E-70012
Diacetoxysuccinic acid, *in* T-70005
1,12-Diacetoxy-4,6-tetradecadiene-8,10-diyne, *in* T-80026
Diacetylacetylene, *see* H-70090
1,5-Diacetylanthracene, D-70028
1,6-Diacetylanthracene, D-70029
1,8-Diacetylanthracene, D-70030
9,10-Diacetylanthracene, D-70031
1,3-Diacetylbicyclo[1.1.1]pentane, D-80041
2,3-Diacetyl-2-butenedioic acid, D-80042
1,1-Diacetylcyclopropane, D-70032
1,2-Diacetyl-1,2-dibenzoylethane, *see* D-60081
Di-2-(7-acetyl-1,4-dihydro-3,6,8-trihydroxy-4,4-dimethyl-1-oxonaphthyl)methane, D-80043
3,6-Diacetyl-1,4,2,5-dioxadiazine, D-80044
3,11-Diacetyl-22-epihippurin 1, *in* E-80039
1,2-Diacetylethylene, *see* H-80084
3,4-Diacetylfurazan, D-80045
▷ 3,4-Diacetylfuroxan, *in* D-80045
3,4-Diacetylfuroxan dioxime, *in* D-80045
▷ 1,3-Diacetylglycerol, D-60023
3,11-Diacetylhippurin-1, *in* E-80039
1,4-Diacetylindole, *in* A-60033
1,3-Diacetyl-5-iodobenzene, D-60024
▷ Diacetylmethane, *see* P-60059
2,3-Di-*O*-acetyltartaric acid, *in* T-70005
7,7′-Diacetyl-1,1′,8,8′-tetrahydroxy-6,6′-dimethyl-2,2′-binaphthyl, *see* S-50130
7,7′-Diacetyl-1′,8,8′-trihydroxy-6,6′-dimethyl[2,2′-binaphthalene]-1,4-dione, *see* I-70003
2,12-Di-9-acridinyl-7-phenyldibenz[*c*,*h*]acridine, D-70033
1,2-Di-1-adamantyl-1,2-di-*tert*-butylethane, *see* D-60025
Di(2-adamantyl) disulfide, *in* A-80038
Di-1-adamantyl selenoketone, D-70034
3,4-Di-1-adamantyl-2,2,5,5-tetramethylhexane, D-60025
Diallyl dicarbonate, *in* D-70111
5,5′-Diallyl-2,2′-dihydroxy-3,3′-dimethoxybiphenyl, *see* D-80023
5,5′-Diallyl-2,2′-dihydroxy-3-methoxybiphenyl, *see* D-80334
1,6-Diallyl-2,5-dithiobiurea, D-60026
Diallyldithiocarbamidohydrazine, *see* D-60026
4′,5-Diallyl-2-hydroxy-2′,3-dimethoxybiphenyl ether, *see* D-80024
Diallyl pyrocarbonate, *in* D-70111
Diallyl tetrasulfide, *see* D-80515
▷ 2,9-Diaminoacridine, D-60027
▷ 3,6-Diaminoacridine, D-60028
▷ 3,9-Diaminoacridine, D-60029
▷ 2,6-Diaminoacridine (obsol.), *see* D-60029
▷ 2,8-Diaminoacridine (obsol.), *see* D-60028
▷ 3,5-Diaminoacridine (obsol.), *see* D-60027
1,4-Diamino-2,3-benzenedithiol, D-60030
2,5-Diamino-1,4-benzenedithiol, D-70035
3,6-Diamino-1,2-benzenedithiol, D-70036
4,6-Diamino-1,3-benzenedithiol, D-70037
1,4-Diamino-2,3,5,6-benzenetetrathiol, D-60031
2,4-Diaminobenzoic acid, D-60032
2,2′-Diaminobiphenyl, D-60033
2,2′-Diamino-4,4′-biphenyldicarboxylic acid, D-80046
4,4′-Diamino-2,2′-biphenyldicarboxylic acid, D-80047
4,4′-Diamino-2,3′-biphenyldicarboxylic acid, D-80048
▷ 4,4′-Diamino-3,3′-biphenyldicarboxylic acid, D-80049
4,6′-Diamino-2,2′-biphenyldicarboxylic acid, D-80050
5,5′-Diamino-2,2′-biphenyldicarboxylic acid, D-80051
6,6′-Diamino-2,2′-biphenyldicarboxylic acid, D-80052
1,5-Diaminobiphenylene, D-80053
2,3-Diaminobiphenylene, D-80054
2,6-Diaminobiphenylene, D-80055
1,8-Diaminocarbazole, D-80056
2,4-Diamino-5-chloropyrimidine, D-80057
▷ 2,4-Diamino-6-chloropyrimidine, D-80058
4,5-Diaminocyclohexene, *see* C-80180
11,12-Diaminodibenzo[*b*,*g*][1,8]naphthyridine, *see* D-80071
2,6-Diamino-1,5-dihydro-4*H*-imidazo[4,5-*c*]pyridin-4-one, D-60034
2,7-Diamino-1,5-dihydro-4,6-pteridinedione, *see* D-60046
2,8-Diamino-1,7-dihydro-6*H*-purin-6-one, D-60035
2,8-Diamino-1,7-dihydro-6*H*-purin-6-one, *see* A-80078
1,3-Diamino-4,6-dimercaptobenzene, *see* D-70037
1,4-Diamino-2,3-dimercaptobenzene, *see* D-60030
1,4-Diamino-2,3-dimercaptobenzene, *see* D-70036
1,4-Diamino-2,5-dimercaptobenzene, *see* D-70035
1,8-Diamino-3,6-dioxaoctane, *see* B-60139
2,2′-Diamino-4,4′-diphenic acid, *see* D-80046
4,4′-Diaminodiphenic acid, *see* D-80047
4,6′-Diaminodiphenic acid, *see* D-80050
5,5′-Diaminodiphenic acid, *see* D-80051
6,6′-Diamino-2,2′-diphenic acid, *see* D-80052
2,7-Diaminodiphenic acid (obsol.), *see* D-80052
1,2-Diamino-1,2-diphenylethane, *see* D-70480
2,6-Diamino-3-heptenedioic acid, D-60036
3,5-Diamino-1-heptyne, *see* H-60026
3,4-Diaminohexanoic acid, D-80059
5,6-Diaminohexanoic acid, D-80060
3,6-Diamino-1-hexyne, *see* H-60080
2,5-Diamino-3-hydroxypentanoic acid, D-70039
2,8-Diamino-6-hydroxypurine, *see* A-80078

2,8-Diamino-6-hydroxypurine, *see* D-60035
2,4-Diamino-6-hydroxypyrimidine, *see* D-70043
2,8-Diaminohypoxanthine, *see* A-80078
2,8-Diaminohypoxanthine, *see* D-60035
2,8-Diaminoinosine, *see* A-70150
4,5-Diaminoisoquinoline, D-70040
5,8-Diaminoisoquinoline, D-70041
3,4-Diamino-1-methoxyisoquinoline, D-60037
1,2-Diamino-4,5-methylenedioxybenzene, D-60038
2,6-Diamino-4-methyleneheptanedioic acid, D-60039
2,5-Diamino-2-methylpentanoic acid, D-80061
2,4-Diamino-6-methyl-1,3,5-triazine, D-60040
1,8-Diaminonaphthalene, D-70042
2-[(2,5-Diamino-1-oxopentyl)amino]ethanesulfonic acid, *see* O-60042
2,4-Diaminopentane, *see* P-70039
▷ 2,4-Diamino-6-phenyl-1,3,5-triazine, D-60041
2,4-Diaminopteridine, D-60042
4,6-Diaminopteridine, D-60043
4,7-Diaminopteridine, D-60044
6,7-Diaminopteridine, D-60045
2,6-Diamino-4,7(3*H*,8*H*)-pteridinedione, D-60047
2,7-Diamino-4,6(3*H*,5*H*)-pteridinedione, D-60046
2,6-Diamino-4(1*H*)-pyrimidinone, D-70043
2,4-Diaminopyrimido[4,5-*b*]pyrazine, *see* D-60042
2,4-Diaminoquinazoline, D-60048
4,5-Diaminoquinoline, D-70044
2,8-Diamino-9-β-D-ribofuranosyl-9*H*-purin-6(1*H*)-one, *see* A-70150
3,4-Diaminotetrahydrofuran, *see* T-70062
1,4-Diamino-2,3,5,6-tetramercaptobenzene, *see* D-60031
3,6-Diamino-1,2,4,5-tetrazine, D-70045
2,5-Diamino-1,3,4-thiadiazole, D-60049
4,6-Diaminothioresorcinol, *see* D-70037
6,10-Diamino-2,3,5-trihydroxydecanoic acid, D-70046
3,5-Diamino-2,4,6-trinitrobenzoic acid, D-70047
1,2:8,9-Dianhydrononitol, *see* D-70465
3,5-Dianilino-1,2,4-thiadiazole, D-70048
Di-9-anthracenylmethanone, D-60050
Dianthramide *A*, D-70049
Dianthramide B, *in* D-70049
Di-9-anthrylacetylene, D-60051
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Diaporthin, D-80062
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2,9-Diazaanthracene, *see* B-80031
Diazaazupyrene, *see* D-70052
9,14-Diazabenz[*a,e*]fluoranthene, *see* D-60069
1,12-Diazabenzo[*a*]phenanthrene, *see* Q-70007
3,4-Diazabenzvalene, *see* D-70054
1,6-Diazabicyclo[3.3.0]decane, *see* O-80016
1,6-Diazabicyclo[4.4.0]decane-2,5-dione, *see* H-70070
2,5-Diazabicyclo[4.1.0]heptane, D-60053
1,4-Diazabicyclo[4.3.0]nonane, D-60054
1,5-Diazabicyclo[4.3.0]nonane, *see* H-70067
▷ 1,4-Diazabicyclo[2.2.2]octane, D-70051
1,5-Diazabicyclo[3.3.0]octane, *see* T-80077
3,7-Diazabicyclo[3.3.0]octane, *see* O-70017
1,5-Diazabicyclo[3.3.0]octane-4,8-dione, *see* T-70087
1,5-Diazabicyclo[5.2.2]undecane, D-60055
4,10-Diaza-15-crown-5, *see* T-60376
4,13-Diaza-18-crown-6, *see* T-60161
1,3-Diazacyclohexane, *see* H-60056
4*a*,8*a*-Diazadecalin, *see* O-80016
▷ 9,14-Diazadibenz[*a,e*]acephenanthrylene, *see* D-60074
5,12-Diazadibenz[*a,h*]anthracene, *see* B-70030
9,14-Diazadibenzo[*a,e*]aceanthrylene, *see* D-60069
10*b*,10*c*-Diazadicyclopenta[*ef,kl*]heptalene, D-70052
3,6-Diazafluorenone, D-70053
3*a*,6-Diazaindene, *see* P-70197
▷ 1,4-Diazaindene, *see* P-60249
2,4-Diazaindene, *see* P-70201
2,5-Diazaindene, *see* P-70200
1,5-Diaza-9-oxa-10-selenaanthracene, *see* O-70065
1,6-Diaza-10-oxa-9-selenaanthracene, *see* O-70068
17-Diaza-10-oxa-9-selenaanthracene, *see* O-70067
1,8-Diaza-10-oxa-9-selenaanthracene, *see* O-70066
1,4-Diazapentalene, *see* D-30286
9,10-Diazaphenanthrene, *see* B-60020
1,6-Diazaphenoxaselenine, *see* O-70065
1,7-Diazaphenoxaselenine, *see* O-70068
1,8-Diazaphenoxaselenine, *see* O-70067
1,9-Diazaphenoxaselenine, *see* O-70066
1,8-Diazaphenoxathiin, *see* O-60050
4,5-Diazapyrene, *see* N-70007
▷ 1,3-Diazaspiro[4.5]decane-2,4-dione, D-60056
1,7-Diazatricyclo[7.3.0.0^{3,7}]decane-2,8-dithione, *see* O-70014
3,4-Diazatricyclo[3.1.0.0^{2,6}]hex-3-ene, D-70054
6,13-Diazatricyclo[10.2.2.2^{5,8}]octadeca-5,7,12,14,15,17-hexaene, *see* P-60228
6,14-Diazatricyclo[10.2.2.2^{5,8}]octadeca-5,7,12,14,15,17-hexaene, *see* P-60227
1,4-Diazaxanthone, *see* B-80035
1,3-Diazetidine-2,4-dione, D-60057
1,2-Diazetidin-3-one, D-70055
3,4-Diazido-3,5-dihydro-thiophene 1,1-dioxide, D-80063
▷ 2,2-Diazido-1,3-indanedione, D-70056
▷ 2,2-Diazido-1*H*-indene-1,3(2*H*)-dione, *see* D-70056
▷ 2,2-Diazidopropane, D-60058
3,4-Diazido-3-sulfolene, *see* D-80063
7-Diazo-7*H*-benzocycloheptene, D-80064
6-Diazo-2,4-cyclohexadien-1-one, D-70057
9-Diazo-9*H*-cyclopenta[1,2-*b*:4,3-*b*′]dipyridine, D-60059
Diazocyclopropane, D-60060
9-Diazo-1,8-diazafluorene, *see* D-60059
Diazodibenzoylmethane, *see* D-70058
2-Diazo-2,3-dihydro-1,1,3,3-tetramethyl-1*H*-indene, *see* D-60067
2-Diazo-1,3-diphenyl-1,3-propanedione, D-70058
1-(1-Diazoethyl)naphthalene, D-60061
9-Diazo-9*H*-fluorene, D-60062
3-Diazo-2,4(5*H*)-furandione, D-70059
▷ 2-Diazo-2*H*-imidazole, D-70060
▷ 4-Diazo-4*H*-imidazole, D-70061
▷ 1,2-Diazole, *see* P-70152
Diazomethanesulfonic acid, D-80065
▷ 1-(Diazomethyl)-4-methoxybenzene, D-60064
1-(Diazomethyl)pyrene, D-70062
▷ 4-Diazo-2-nitro-2,5-cyclohexadien-1-one, *see* D-60065
▷ 4-Diazo-2-nitrophenol, D-60065
6-Diazo-5-oxo-1,3-cyclohexadiene-1-carboxylic acid, D-70063
o-Diazophenol, *see* D-70057
2-Diazopropanal, D-80066
2-Diazo-1,1,3,3-tetramethylcyclopentane, D-60066
2-Diazo-2,2,6,6-tetramethyl-3,5-heptanedione, D-70064
2-Diazo-1,1,3,3-tetramethylindane, D-60067
3-Diazotetronic acid, *see* D-70059
9-Diazo-9*H*-thioxanthene, D-70065
Dibenz[*e,k*]acephenanthrylene, D-70066
Dibenz[*a,h*]anthracene-5,6:11,12-dioxide, *see* D-70151
Dibenz[*b,g*]azocine-5,7(6*H*,12*H*)-dione, D-60068
3,4:7,8-Dibenz-2,6,9-bisdioxan, *see* D-70505
1,2,3,4-Dibenzcyclohepta-1,3-diene-6-one, *see* D-70187
1,2,3,4-Dibenzcyclohepta-1,3-dien-5-one, *see* D-70188
o,o′-Dibenzene, *see* T-60060
sym-Dibenzfulvalene, *see* B-60109
Dibenzhydrylamine, *see* T-70150
13*H*-Dibenzimidazo[2,1-*b*:1′,2′-*e*][1,3,5]thiadiazine-13-thione, *see* T-60191
Dibenz[*b,h*]indeno[1,2,3-*de*][1,6]naphthyridine, D-60069
2*H*-Dibenz[*e,g*]isoindole, D-70067
2,3;6,7-Dibenzobicyclo[3.3.1]nona-2,6-diene-4,8-dione, *see* M-80040
Dibenzobicyclo[2.2.2]octadiene, *see* D-70207
11*H*-Dibenzo[*a,def*]carbazole, D-80067
Dibenzo[*c,g*]carbazole-6-carboxylic acid, D-80068
Dibenzo[*a*,cd]naphtho[1,2,3-*lm*]perylene, *see* B-60037
Dibenzo-12-crown-4, *see* T-80059
Dibenzo-54-crown-18, D-70068
Dibenzocyclohepta-1,3-diene, *see* D-70186
Dibenzo[*a,c*][1,3]cycloheptadien-5-one, *see* D-70188
Dibenzo[*a,d*]cycloheptenylium, D-60071
Dibenzo[*jk,uv*]dinaphtho[2,1,8,7-*defg*:2′,1′,8′,7′-*opqr*]pentacene, D-60072
3,3′-Dibenzo[*b,e*][1,4]dioxin-2,8-diylbis[5-hydroxy-8,8-dimethyl-6-(3-methyl-2-butenyl)-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one], *see* D-80517
6*H*,12*H*-Dibenzo[*b,f*][1,5]dithiocin, D-70070
5*H*,7*H*-Dibenzo[*b,g*][1,5]dithiocin, D-70069
1,2-Di-(1-Benzofuranyl)ethylene, D-80069
Dibenzo[*f,h*]furo[2,3-*b*]quinoline, D-80070
4,5:15,16-Dibenzo-3,6,14,17,23,24-hexaazatricyclo[17.3.1.1^{8,12}]tetracosa-1(23),4,8(24),9,11,15,19,21-octaene, *see* D-60456
2,3,11,12-Dibenzo-1,4,7,10,13,16-hexathia-2,11-cyclooctadecadiene, D-60073
▷ Dibenzo[*c,f*]indeno[1,2,3-*ij*][2,7]naphthyridine, D-60074
1,2:9,10-Dibenzo[2.2]metaparacyclophane, D-70071
Dibenzo[*a,rst*]naphtho[8,1,2-*cde*]pentaphene, D-60075
Dibenzo[*b,g*][1,8]naphthyridine-11,12-diamine, D-80071
Dibenzo[*fg,mn*]octalene, D-80072
1,2:7,8-Dibenzo[2.2]paracyclophane, D-70072
1,2:9,10-Dibenzo[2.2]paracyclophanediene, *see* D-70072
1,2;5,6-Dibenzopentafulvalene, *see* B-60109
Dibenzo[*fg,ij*]pentaphene-15,16-dione, D-80073
Dibenzo[*a,j*]perylene-8,16-dione, D-70073
1,2:7,8-Dibenzoperylene-3,9-quinone, *see* D-70073
Dibenzo[2,3:10,11]perylo[1,12-*bcd*]thiophene, D-70074
Dibenzo[*f,h*]quinoline, D-70075
Dibenzo[*a,h*]quinolizinium(1+), D-70076
5*H*,7*H*-Dibenzo[*c,e*]selenepin, *see* D-70189
Dibenzosemibullvalene, *see* T-80057
2,3:6,7-Dibenzosuberane, *see* D-60217
Dibenzotetraselenofulvalene, D-70077
Dibenzo[*cd*:*c*′*d*′][1,2,4,5]tetrazino[1,6-*a*:4,3-*a*′]diindole, D-60076
Dibenzo[*b,i*]thianthrene-5,7,12,14-tetrone, D-70078
Di-2-benzothiazolylamine, D-80074
Dibenzo[*f,h*]thieno[2,3-*b*]quinoline, D-70079
Dibenzo[*b,f*]thiepin-3-carboxylic acid, D-60077
Dibenzo[*b,f*]thiepin-3-methanol, *see* H-60176
Dibenzo[*b,e*]thiepin-11(6*H*)-one, D-80075
Dibenzo[*b,f*]thiepin-10(11*H*)-one, D-80076
2-Dibenzothiophenethiol, D-60078
4-Dibenzothiophenethiol, D-60079
6*H*-Dibenzo[*b,d*]thiopyran-6-one, D-70080
Dibenzo[*b,d*]thiopyrylium(1+), D-70081
Dibenzotricyclo[3.3.0.0^{2,8}]octa-3,6-diene, *see* T-80057
2,3:7,8-Dibenzotricyclo[4.4.1.0^{1,6}]undeca-4,9-diene, *see* M-70040

Dibenzo[*b,m*]triphenodithiazine-5,7,9,14,16,18(8*H*,17*H*)-tetrone, D-70082
7*H*-Dibenzo[*c,h*]xanthen-7-one, D-60080
1,3-Dibenzoylacetone, *see* D-60489
2,3-Dibenzoylbutanedioic acid, D-70083
2,3-Dibenzoyl-1,4-diphenyl-1,4-butanedione, *see* T-60020
2,3-Dibenzoyl-1,4-diphenyl-2-butene-1,4-dione, *see* T-60021
3,4-Dibenzoyl-2,5-hexanedione, D-60081
2,3-Dibenzoylsuccinic acid, *see* D-70083
2,3-Di-*O*-benzoyltartaric acid, *in* T-70005
2,3:10,11-Dibenzperylene-1,12-quinone (obsol.), *see* D-80073
Dibenz[*a,g*]pyracyclene, *see* I-80010
Dibenzyl dicarbonate, *in* D-70111
1,3-Dibenzyl-1,3-dihydroisoindole, D-80077
1,4-Dibenzyl-6,7-dihydroxy-1,4-diazocane-5,8-dione, D-80078
Dibenzyl diselenide, D-60082
N,N'-Dibenzyl-*N,N'*-ethylenetartramide, *see* D-80078
1,2-Dibenzylidenecyclobutane, D-60083
1,3-Dibenzylisoindoline, *see* D-80077
Dibenzyl pyrocarbonate, *in* D-70111
1,3-Dibromoadamantane, D-70084
2,3-Dibromoanthracene, D-70085
9,10-Dibromoanthracene, D-60085
ms-Dibromoanthracene, *see* D-60085
2,3-Dibromobenzofuran, D-60086
5,7-Dibromobenzofuran, D-60087
1,2-Dibromobenzonorbornadiene, *see* D-60095
1,3-Dibromobenzonorbornadiene, *see* D-60096
2,6-Dibromo-1,4-benzoquinone, D-60088
α,α'-Dibromobibenzyl, *see* D-70091
1,4-Dibromobicyclo[2.2.2]octane, D-70086
2,2'-Dibromo-1,1'-binaphthalene, *see* D-60089
4,4'-Dibromo-1,1'-binaphthalene, *see* D-60090
2,2'-Dibromo-1,1'-binaphthyl, D-60089
4,4'-Dibromo-1,1'-binaphthyl, D-60090
1,5-Dibromo-3,3-bis(2-bromoethyl)pentane, *see* T-70124
1,1-Dibromo-2,2-bis(chloromethyl)cyclopropane, D-80079
2,4-Dibromobutanoic acid, D-80080
▷ 1,4-Dibromo-2-butyne, D-70087
2,10-Dibromo-3-chloro-7-chamigren-9-ol, D-80081
1,1-Dibromo-2-chlorocyclopropane, D-80082
4,10-Dibromo-3-chloro-7,8-epoxy-9-hydroxy-α-chamigrane, D-80083
7,8-Dibromo-6-(chloromethylene)-2-methyl-2-octene, D-70088
▷ 1,1-Dibromo-1-chloro-2,2,2-trifluoroethane, D-80084
1,2-Dibromo-1-chloro-1,2,2-trifluoroethane, D-80085
2,3-Dibromocoumarone, *see* D-60086
5,7-Dibromocoumarone, *see* D-60087
1,1-Dibromocycloheptane, D-60091
2,6-Dibromo-2,5-cyclohexadiene-1,4-dione, *see* D-60088
2,2-Dibromocyclopropanecarboxaldehyde, D-60092
2,2-Dibromocyclopropanecarboxylic acid, D-60093
1,2-Dibromocyclopropene, D-60094
α,β-Dibromodibenzyl, *see* D-70091
Dibromodi-*tert*-butylmethane, *see* D-80104
4,8-Dibromo-3,7-dichloro-3,7-dimethyl-1,5-octadiene, D-80086
9,13-Dibromo-6,12;7,10-diepoxypentadec-3-en-1-yne, *see* I-70067
1,2-Dibromo-4,5-difluorobenzene, D-80087
1,4-Dibromo-2,5-difluorobenzene, D-80088
1,2-Dibromo-1,4-dihydro-1,4-methanonaphthalene, D-60095
1,3-Dibromo-1,4-dihydro-1,4-methanonaphthalene, D-60096
2,2-Dibromo-2,3-dihydro-1,1,3,3-tetramethyl-1*H*-indene, D-80089
2,6-Dibromo-4,5-dihydroxy-2-cyclohexen-1-one, D-60097
3,5-Dibromo-1,6-dihydroxy-4-oxo-2-cyclohexene-1-acetonitrile, D-60098
4,5-Dibromo-3,6-diiodo-1,2-benzenediol, D-80090
4,5-Dibromo-3,6-diiodocatechol, *see* D-80090
1,2-Dibromo-3,6-diiodo-4,5-dimethoxybenzene, *in* D-80090
4,5-Dibromo-3,6-diiodoveratrole, *in* D-80090
1,1-Dibromo-3,3-dimethoxy-2-methyl-1-butene, *in* D-70094
1,3-Dibromo-2,3-dimethylbutane, D-70089
1,5-Dibromo-3,3-dimethylpentane, D-70090
2,4-Dibromo-2,4-dimethyl-3-pentanone, D-60099
2,2'-Dibromo-3,5'-dinitrobiphenyl, D-80091
2,2'-Dibromo-5,5'-dinitrobiphenyl, D-80092
5,5'-Dibromo-2,2'-dinitrobiphenyl, D-80093
2,2'-Dibromodiphenylacetylene, *see* B-80140
4,4'-Dibromodiphenylacetylene, *see* B-80141
1,2-Dibromo-1,2-diphenylethane, D-70091
1,1'-(1,2-Dibromo-1,2-ethanediyl)bisbenzene, *see* D-70091
3-(2,2-Dibromoethenyl)-2,2-dimethylcyclopropanecarboxylic acid cyano(3-phenoxyphenyl)methyl ester, *see* D-80027
4,21-Dibromo-3-ethyl-2,19-dioxabicyclo[16.3.1]docosa-6,9,18(22),21-tetraen-12-yn-20-one, *in* E-70042
1,3-Dibromo-1,1,2,2,3,3-hexafluoropropane, D-80094
1,6-Dibromo-3,4-hexanediol, D-80095
2,4-Dibromo-6-hydroxypyridine, *see* D-80100
2,6-Dibromo-4-hydroxypyridine, *see* D-80099
1,20-Dibromoicosane, D-70092
2,4(5)-Dibromo-1*H*-imidazole, D-70093
4,5-Dibromo-1*H*-imidazole, D-60100
4,5-Dibromo-2-formyl-1*H*-imidazole, *see* D-60101
4,5-Dibromo-1*H*-imidazole-2-carboxaldehyde, D-60101
4,5-Dibromo-1*H*-imidazole-2-carboxylic acid, D-60102
2,4-Dibromo-6-methoxypyridine, *in* D-80100
2,6-Dibromo-4-methoxypyridine, *in* D-80099
1,3-Dibromo-2-methylbenzene, D-60103
1,1-Dibromo-3-methyl-1-butene, D-60104
4,4-Dibromo-3-methyl-3-buten-2-one, D-70094
4,5-Dibromo-6-methyl-1,2,3-triazine, D-80096
6,7-Dibromo-1-naphthalenamine, *see* D-70097
6,7-Dibromo-1,4-naphthalenedione, *see* D-70096
6,7-Dibromo-1-naphthalenol, *see* D-70095
6,7-Dibromo-1-naphthol, D-70095
6,7-Dibromo-1,4-naphthoquinone, D-70096
6,7-Dibromo-1-naphthylamine, D-70097
6,7-Dibromo-1-nitronaphthalene, D-70098
2,3-Dibromo-5-nitronaphthalene (incorr.), *see* D-70098
2,6-Dibromo-4-nitroso-1-naphthol, *in* D-60088
ω,ω'-Dibromo-5-nitro-*m*-xylene, *see* B-60145
4,5-Dibromo-6-phenyl-1,2,3-triazine, D-80097
▷ 1,2-Dibromopropane, D-60105
1,8-Dibromopyrene, D-70099
4,9-Dibromopyrene, D-80098
2,6-Dibromo-4(1*H*)-pyridone, D-80099
4,6-Dibromo-2(1*H*)pyridone, D-80100
1,2-Dibromo-3,4,5,6-tetrafluorobenzene, D-60106
1,3-Dibromo-2,4,5,6-tetrafluorobenzene, D-60107
1,4-Dibromo-2,3,5,6-tetrafluorobenzene, D-60108
2,2-Dibromo-1,1,3,3-tetramethylcyclohexane, D-80101
2,2-Dibromo-1,1,3,3-tetramethylcyclopentane, D-80102
1,1-Dibromo-2,2,3,3-tetramethylcyclopropane, D-80103
2,2-Dibromo-1,1,3,3-tetramethylindane, *see* D-80089
3,3-Dibromo-2,2,4,4-tetramethylpentane, D-80104
2,4-Dibromothiazole, D-60109
2,5-Dibromothiazole, D-60110
4,5-Dibromothiazole, D-60111
2,2'-Dibromotolan, *see* B-80140
4,4'-Dibromotolan, *see* B-80141
2,6-Dibromotoluene, *see* D-60103
4,5-Dibromo-1,2,3-triazine, D-70100
4,5-Dibromo-1,2,3-triazine, D-80105
1,3-Dibromotricyclo[3.3.1.1^{3,7}]decane, *see* D-70084
2,2-Dibromo-1,1,1-trifluoroethane, D-80106
1,11-Dibromo-6-undecanone, D-80107
Dibusadol, *in* H-70108
2,3-Di-*tert*-butoxycyclopropenone, *in* D-70290
1,3-Dibutylallene, *see* T-60272
1,3-Dibutylallene, *see* U-80016
2,3-Di-*tert*-butyl-1,3-butadiene, D-80108
Di-*tert*-butylcarbinol, *see* T-80148
1,1-Di-*tert*-butylcyclopropane, D-60112
3,6-Di-*tert*-butyl-1,4-diazapentalene, *see* D-70108
2,2-Di-*tert*-butyl-3-(di-*tert*-butylmethylene)cyclopropanone, D-70101
Di-*tert*-butyl dicarbonate, *in* D-70111
Di-*tert*-butyldichloromethane, *see* D-80137
2,7-Di-*tert*-butyldicyclopenta[*a,e*]cyclooctene, D-70102
2,5-Di-*tert*-butyl-2,5-dihydrobenzo[*e*]pyrrolo[3,4-*g*]isoindole, D-70103
2,7-Di-*tert*-butyl-2,7-dihydroisoindolo[5,4-*e*]isoindole, D-70104
Di-*tert*-butyl diketone, *see* T-80146
Di-*sec*-butyldiketopiperazine, *see* B-70153
3,7-Di-*tert*-butyl-9,10-dimethyl-2,6-anthraquinone, D-60113
2,6-Di-*tert*-butyl-1-nitronaphthalene, D-80109
3,7-Di-*tert*-butyl-1-nitronaphthalene, D-80110
5-(3,5-Di-*tert*-butyl-4-oxo-2,5-cyclohexadienylidene)-3,6-cycloheptadiene-1,2-dione, D-70105
Di-*tert*-butyl pentaketone, *see* T-60148
2,6-Di-*tert*-butylpiperidine, D-80111
3,4-Di-*tert*-butylpyrazole, D-70106
3,5-Di-*tert*-butylpyrazole, D-70107
Di-*tert*-butyl pyrocarbonate, *in* D-70111
3,6-Di-*tert*-butylpyrrolo[3,2-*b*]pyrrole, D-70108
3,4-Di-*tert*-butyl-2,2,5,5-tetramethylhexane, D-70109
Di-*tert*-butylthioketene, D-60114
2,4-Di-*tert*-butylthiophene, D-80112
3,4-Di-*O*-caffeoylquinic acid, D-70110
▷ Dicarbamide, *see* T-70097
2,2'-Dicarbamoyldiphenylamine, *in* I-60014
1,4-Dicarbomethoxyazulene, *in* A-70293
2,3-Dicarbomethoxy-1,3-butadiene, *in* D-70409
Dicarbon dioxide, D-80114
Dicarbonic acid, D-70111
6-(1,2-Dicarboxyethylamino)purine, D-80115
α-Diceroptene, D-70112
4,5-Dichloro-2-formylimidazole, *see* D-60134
5,6-Dichloroacenaphthene, D-60115
4,5-Dichloroacenaphthene (obsol.), *see* D-60115
α,β-Dichloroacrolein, *see* D-80127
▷ β,β-Dichloroacrolein, *see* D-80128
9,10-Dichloroanthracene, D-60116
ms-Dichloroanthracene, *see* D-60116
2,3-Dichloro-1,4,9,10-anthracenetetrone, D-60117
4,6-Dichloro-1,3-benzenedicarboxaldehyde, D-60118
2,3-Dichlorobenzenethiol, D-60119
2,4-Dichlorobenzenethiol, D-60120
2,5-Dichlorobenzenethiol, D-60121
2,6-Dichlorobenzenethiol, D-60122
3,4-Dichlorobenzenethiol, D-60123

3,5-Dichlorobenzenethiol, D-60124
2,2-Dichloro-1,3-benzodioxole, D-70113
2,3-Dichlorobenzofuran, D-60125
5,7-Dichlorobenzofuran, D-60126
1,4-Dichlorobenzo[*g*]phthalazine, D-70114
1,4-Dichlorobicyclo[2.2.2]octane, D-70115
1,8-Dichloro-6-chloromethyl-2-methyl-2,6-octadiene, D-70116
3,8-Dichloro-6-chloromethyl-2-methyl-1,6-octadiene, D-70117
1,3-Dichloro-2-(chloromethyl)propane, D-70118
2,3-Dichlorocoumarone, *see* D-60125
5,7-Dichlorocoumarone, *see* D-60126
2,2-Dichlorocyclopropanecarboxylic acid, D-60127
2,3-Dichloro-5,6-dicyanopyrazine, *in* D-80129
2,2′-Dichlorodiethyl ketone, *see* D-80125
2,2-Dichloro-3,3-difluorooxirane, D-60128
5,6-Dichloro-1,2-dihydroacenaphthylene, *see* D-60115
2,4-Dichloro-1,8-dihydroxy-5-methoxy-6-methylxanthone, *see* T-70181
1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone, D-60129
3,5-Dichloro-2,4-dihydroxy-6-methylbenzoic acid 4-carbomethoxy-3-hydroxy-5-methylphenyl ester, *see* T-70334
4,6-Dichloro-5-[(dimethylamino)methylene]-3,6-cyclohexadiene-1,3-dicarboxaldehyde, D-70119
2,4-Dichloro-3,4-dimethyl-2-cyclobuten-1-one, D-60130
4,4-Dichloro-2,3-dimethyl-2-cyclobuten-1-one, D-60131
1,1-Dichloroepoxy-2,2-difluoroethane, *see* D-60128
▷ 1,1-Dichloroethene, *see* D-80116
▷ 1,1-Dichloroethylene, D-80116
Di(2-chloroethyl) ketone, *see* D-80125
1,1-Dichloro-1-fluoroethane, D-80117
1,1-Dichloro-2-fluoroethene, D-80118
2,3-Dichloro-*N*-(4-fluorophenyl)maleimide, *see* D-60132
3,4-Dichloro-1-(4-fluorophenyl)-1*H*-pyrrole-2,5-dione, D-60132
3′,6-Dichlorogenistein, *see* D-80147
2,2-Dichloro-6-heptenoic acid, D-80119
1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane, D-80120
1,3-Dichloro-1,1,2,2,3,3-hexafluoropropane, D-80121
2,2-Dichloro-1,1,1,3,3,3-hexafluoropropane, D-80122
2,5-Dichloro-4-hydroxybenzaldehyde, D-70120
2,6-Dichloro-4-hydroxybenzaldehyde, D-70121
2,3-Dichloro-4-hydroxybenzoic acid, D-60133
2,4-Dichloro-1-hydroxy-5,8-dimethoxyxanthone, *in* T-70181
4,6-Dichloro-2-hydroxypyrimidine, *see* D-80131
4,5-Dichloro-1*H*-imidazole, D-70122
4,5-Dichloro-1*H*-imidazole-2-carboxaldehyde, D-60134
4,5-Dichloro-1*H*-imidazole-2-carboxylic acid, D-60135
5,6-Dichloro-1*H*-indole-3-acetic acid, D-70123
3,3′-Dichloroisobutylene, *see* C-70061
4,6-Dichloroisophthalaldehyde, *see* D-60118
6,7-Dichloroisoquinoline, D-60136
6,7-Dichloro-5,8-isoquinolinedione, D-60137
1,2-Dichloro-3-mercaptobenzene, *see* D-60119
1,2-Dichloro-4-mercaptobenzene, *see* D-60123
1,3-Dichloro-2-mercaptobenzene, *see* D-60122
1,3-Dichloro-5-mercaptobenzene, *see* D-60124
1,4-Dichloro-2-mercaptobenzene, *see* D-60121
2,4-Dichloro-1-mercaptobenzene, *see* D-60120
2,6-Dichloro-4-methoxybenzaldehyde, *in* D-70121
2,3-Dichloro-4-methoxybenzoic acid, *in* D-60133
2,3-Dichloro-1-methoxy-4-nitrobenzene, *in* D-70125
1,2-[(Dichloromethylene)dioxy]benzene, *see* D-70113
2,3-Dichloro-5-methylpyridine, D-60138
2,5-Dichloro-3-methylpyridine, D-60139
1,2-Dichloro-4-(methylthio)benzene, *in* D-60123
1,4-Dichloro-2-(methylthio)benzene, *in* D-60121
6,7-Dichloro-1,4-naphthalenedione, *see* D-70124
6,7-Dichloro-1,4-naphthoquinone, D-70124
2,3-Dichloro-4-nitroanisole, *in* D-70125
2,3-Dichloro-4-nitrophenol, D-70125
2,3-Dichloro-5-nitropyridine, D-60140
2,4-Dichloro-3-nitropyridine, D-60141
2,4-Dichloro-5-nitropyridine, D-60142
2,5-Dichloro-3-nitropyridine, D-60143
2,6-Dichloro-3-nitropyridine, D-60144
2,6-Dichloro-4-nitropyridine, D-60145
3,4-Dichloro-5-nitropyridine, D-60146
3,5-Dichloro-4-nitropyridine, D-60147
1,1-Dichlorooctane, D-70126
1,2-Dichlorooctane, D-70127
1,3-Dichlorooctane, D-70128
2,2-Dichlorooctane, D-70129
2,3-Dichlorooctane, D-70130
4,5-Dichlorooctane, D-70131
2,2-Dichloro-7-octenoic acid, D-80123
1,5-Dichloro-3-pentanol, D-80124
1,5-Dichloro-3-pentanone, D-80125
2,5-Dichloro-1-pentene, D-80126
1,4-Dichlorophenanthrene, D-70132
2,4-Dichlorophenanthrene, D-70133
3,6-Dichlorophenanthrene, D-70134
3,9-Dichlorophenanthrene, D-70135
4,5-Dichlorophenanthrene, D-70136
9,10-Dichlorophenanthrene, D-70137
2,3-Dichlorophenylalanine, *see* A-60127
2,4-Dichlorophenylalanine, *see* A-60128
2,5-Dichlorophenylalanine, *see* A-60129
2,6-Dichlorophenylalanine, *see* A-60130
3,4-Dichlorophenylalanine, *see* A-60131
3,5-Dichlorophenylalanine, *see* A-60132
4-[(2,5-Dichlorophenyl)azo]-2,4-dihydro-5-methyl-2-phenyl-3*H*-pyrazol-3-one, *see* D-70138
4-(2,5-Dichlorophenylhydrazono)-5-methyl-2-phenyl-3*H*-pyrazol-3-one, D-70138
2,3-Dichlorophenyl mercaptan, *see* D-60119
2,4-Dichlorophenyl mercaptan, *see* D-60120
2,5-Dichlorophenyl mercaptan, *see* D-60121
2,6-Dichlorophenyl mercaptan, *see* D-60122
3,4-Dichlorophenyl mercaptan, *see* D-60123
3,5-Dichlorophenyl mercaptan, *see* D-60124
1,4-Dichlorophthalazine, D-60148
2,5-Dichloro-3-picoline, *see* D-60139
5,6-Dichloro-3-picoline, *see* D-60138
2,3-Dichloro-2-propenal, D-80127
▷ 3,3-Dichloro-2-propenal, D-80128
5,6-Dichloro-2,3-pyrazinedicarboxylic acid, D-80129
2,6-Dichloro-4(3*H*)-pyrimidinone, D-80130
4,6-Dichloro-2(1*H*)-pyrimidinone, D-80131
6,7-Dichloro-5,8-quinolinedione, D-60149
▷ 2,3-Dichloroquinoxaline, D-60150
1,2-Dichloro-3,4,5,6-tetrafluorobenzene, D-60151
1,3-Dichloro-2,4,5,6-tetrafluorobenzene, D-60152
1,4-Dichloro-2,3,5,6-tetrafluorobenzene, D-60153
1,2-Dichloro-3,3,4,4-tetrafluorocyclobutene, D-80132
3,4-Dichloro-1,2,3,4-tetrafluorocyclobutene, D-80133
▷ 1,1-Dichloro-1,2,2,2-tetrafluoroethane, D-80134
1,1-Dichloro-2,3,3,3-tetrafluoro-1-propene, D-80135
1,2-Dichloro-1,3,3,3-tetrafluoro-1-propene, D-80136
3,3-Dichloro-2,2,4,4-tetramethylpentane, D-80137
2,4-Dichlorothiazole, D-60154
2,5-Dichlorothiazole, D-60155
4,5-Dichlorothiazole, D-60156
2,5-Dichlorothioanisole, *in* D-60121
3,4-Dichlorothioanisole, *in* D-60123
2,3-Dichlorothiophenol, *see* D-60119
2,4-Dichlorothiophenol, *see* D-60120
2,5-Dichlorothiophenol, *see* D-60121
2,6-Dichlorothiophenol, *see* D-60122
3,4-Dichlorothiophenol, *see* D-60123
3,5-Dichlorothiophenol, *see* D-60124
1,4-Dichloro-3,3,4-trifluorocyclobutene, D-80138
1,1-Dichloro-1,2,2-trifluoroethane, D-80139
▷ 1,2-Dichloro-1,1,2-trifluoroethane, D-80140
2,2-Dichloro-1,1,1-trifluoroethane, D-80141
▷ 1,1-Dichloro-1,2,2-trifluoro-2-iodoethane, D-80142
1,2-Dichloro-1,1,2-trifluoro-2-iodoethane, D-80143
▷ 4,5-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60157
▷ 4,6-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60158
▷ 4,7-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60159
▷ 5,6-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60160
2,2-Dichloro-1,1,1-trifluoropropane, D-80144
2,3-Dichloro-1,1,1-trifluoropropane, D-80145
3,3-Dichloro-1,1,1-trifluoropropane, D-80146
2,2-Dichloro-3,3,3-trifluoro-1-propanol, D-60161
3′,6-Dichloro-4′,5,7-trihydroxyisoflavone, D-80147
1,5-Dichloro-9*H*-xanthen-9-one, *see* D-70139
1,7-Dichloro-9*H*-xanthen-9-one, *see* D-70140
2,6-Dichloro-9*H*-xanthen-9-one, *see* D-70141
2,7-Dichloro-9*H*-xanthen-9-one, *see* D-70142
3,6-Dichloro-9*H*-xanthen-9-one, *see* D-70143
1,5-Dichloroxanthone, D-70139
1,7-Dichloroxanthone, D-70140
2,6-Dichloroxanthone, D-70141
2,7-Dichloroxanthone, D-70142
3,6-Dichloroxanthone, D-70143
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Dicranolomin, D-70144
Dictymal, D-60162
Dictyoceratin, D-80148
Dictyodendrillolide, D-80149
Dictyodial *A*, D-70145
Dictyone, D-70146
Dictyotriol *A*, D-70147
Dictytriene *A*, D-70148
Dictytriene *B*, *in* D-70148
Dictytriol, *in* D-70148
Dicyanic acid, *see* D-60057
5,6-Dicyanoacenaphthene, *in* A-70015
Dicyanoacetic acid, D-70149
1,8-Dicyanoanthracene, *in* A-60281
5,7-Dicyanoazulene, *in* A-70295
2,2′-Dicyanobibenzyl, *in* B-80071
1,1′-Dicyanobicyclopropyl, *in* B-70114
5,5′-Dicyano-2,2′-bipyridine, *in* B-60127
2,3-Dicyano-1,3-butadiene, *in* D-70409
2,4-Dicyano-1-butene, *see* M-80089
1,1-Dicyanocyclopropane, *in* C-80196
4,4′-Dicyanodiphenylamine, *in* I-60018
1,1-Dicyanoethane, *in* M-80149
2,2-Dicyanoethylene-1,1-dithiol, *in* D-60395
2,3-Dicyano-1-methoxy-4-nitrobenzene, *in* H-70189
9-(Dicyanomethyl)anthracene, D-60163
10-(Dicyanomethyl)-9(10*H*)-anthracenone, *see* D-60164
[10-[(10-Dicyanomethylene)-9(10*H*)-anthracenylidene]-9(10*H*)-anthracenylidene]propanedinitrile, *see* T-60030
10-(Dicyanomethylene)anthrone, D-60164
2,3-Dicyanonaphthalene, *in* N-80001

1,5-Dicyano-3-pentanone, *in* O-60071
3,6-Dicyano-1,2,4,5-tetrazine, *in* T-80163
Dicyanotriselenide, D-60165
Dicyclobuta[1,4]dithiin-1,2,4,5-tetraone, *see* D-60506
Di(1,3,5-cycloheptatrien-3-yl)(2,4,6-cycloheptatrienylidene)methane, *see* C-60205
Di(2,4,6-cycloheptatrien-1-yl)ethanone, D-60166
Di(2,4,6-cycloheptatrien-1-yl) ketone, *see* D-60166
Dicyclohexylcarbinol, *see* D-70150
1,2:5,6-Di-*O*-cyclohexylidene-*myo*-inositol, *in* I-80015
Dicyclohexylmethanol, D-70150
Dicyclopenta[*ef*,*kl*]heptalene, D-60167
Dicyclopropyldiazene, *see* A-80205
Dicyclopropylmethanethione, D-80150
Dicyclopropyl thioketone, *see* D-80150
2,3-Didehydro-1,2-dihydro-1,1-dimethylnaphthalene, D-60168
(9′*E*)-3′,4′-Didehydro-1′,2′-dihydro-3*R*-hydroxy-1′-methoxy-*β*,*ψ*-caroten-19′-al, *in* D-80151
3′,4′-Didehydro-1′,2′-dihydro-1′-methoxy-*β*,*ψ*-caroten-3-ol, D-80151
5,6-Didehydro-2,7-dihydroxytaxodone, *see* T-80085
12,13-Didehydrofurospongin I, *in* F-80097
1,16-Didehydrohexahelicene, *see* H-80037
3,7-Didehydrojasmonic acid, *see* O-80090
2,3-Didehydronorleucine, *see* A-60167
1,5-Didehydroproline, *see* D-80248
5,6-Didehydropygmaeocin A, *in* P-80195
3,4-Didehydropyridine, *see* P-80224
1,10-Didehydro-2-quinolizidone, *see* H-60059
Didehydrorotenone, *see* D-80026
N,6-Didehydro-1,2,3,6-tetrahydro-1-methyl-2-oxoadenosine, *see* D-60518
7,8-Didehydro-3,4,5,6-tetrahydro-2*H*-thiocin, *see* T-60189
5,6-Didehydro-1,4,7,10-tetramethyldibenzo[*ae*]cyclooctene, D-60169
4,5-Didehydrotropone, *see* C-60196
Didemethoxyaaptamine, *see* B-70037
▷ 6,27-Didemethoxyantibiotic *A* 204*A*, *see* C-60022
▷ 16,34-Didemethyl-21,27,29,31-tetradeoxy-12,13,32,33-tetrahydro-13-hydroxy-2-methyl-21,27-dioxodermostatin *A*, *see* R-70009
2′,3′-Dideoxy-5-azacytidine, *in* A-80149
2′,3′-Dideoxycytidine, D-80152
15,16-Dideoxy-15,17-dihydroxy-15,17-oxido-16-spongianoic acid, *see* T-60038
1,2-Dideoxy-2-(hydroxymethyl)-D-*chiro*-inositol, *in* H-70170
2,3-Dideoxy-2-(hydroxymethyl)-D-*epi*-inositol, *in* H-70170
2,3-Dideoxy-3-(hydroxymethyl)-D-*myo*-inositol, *in* H-70170
1,6-Dideoxy-1-(hydroxymethyl)-L-*chiro*-inositol, *in* H-70170
2,5-Dideoxy-*γ*-pentonolactone, *in* D-80353
Dieckmann ester, *in* O-70084
Diepiserratenediol, *in* S-80027
21,23*R*:24*S*,25-Diepoxyapotirucall-14-ene-3α,7α,21*S*-triol, *see* T-60223
2,16:11,12-Diepoxy-1(15),8*E*,12*E*-cembratriene, *see* I-70100
2,16;7,8-Diepoxy-1(15),3,11-cembratriene, *see* S-70011
ent-3*β*,4*β*;15,16-Diepoxy-13(16),14-clerodadien-2*β*-ol, D-80153
4*β*,6*β*;15,16-Diepoxy-2*β*-hydroxy-13(16),14-clerodadiene-18,19;20,12*S*-diolide, *see* C-60032
1*β*,10α; 4α,5*β*-Diepoxy-8α-isobutoxyglechomanolide, *in* G-60022
1*β*,10α; 4α,5*β*-Diepoxy-8*β*-isobutoxyglechomanolide, *in* G-60022
ent-3*β*,4*β*;15,16-Diepoxy-2*β*-methoxy-13(16),14-clerodadiene, *in* D-80153
5,6:12,13-Diepoxy-5,6,12,13-tetrahydrodibenz[*a*,*h*]anthracene, D-70151
4,5:9,10-Diepoxy-4,5,9,10-tetrahydropyrene, D-70152
4,7:12,15-Diethenobenzo[7,8]cyclododeca[1,2-*c*]furan, D-80154
6,9:14,17-Diethenobenzo[7,8]cyclododeca[1,2-*b*]naphthalene, *see* B-80029
5,8:11,14-Diethenobenzocyclododecene, *see* B-80033
5,8:13,16-Diethenodibenzo[*a*,*g*]cyclododecene, *see* D-70072
1,3-Diethenyltricyclo[3.3.1.1^{3,7}]decane, *see* D-70529
Diethoxyacetaldehyde, D-70153
4,4-Diethoxybutanenitrile, *in* O-80068
1,1-Diethoxy-2-butanone, *in* O-80067
4,4-Diethoxybutylamine, *in* A-80064
4,4-Diethoxy-2-butynal, *in* B-60351
2,7-Diethoxycycloheptene, *in* C-80179
3,6-Diethoxycyclohexene, *in* C-80181
4,6-Diethoxy-2,5-dihydropyrimidine, *in* D-70256
1,5-Diethoxy-2,4-dinitrobenzene, *in* D-80491
2,2-Diethoxyethanethiol, *in* M-80017
3,4-Diethoxy-1,5-hexadiene, *in* H-70036
2,5-Diethoxy-3-hexene, *in* H-80083
4,4-Diethoxy-2-methyl-2-butene, *in* M-70055
1,1-Diethoxy-2-methylenecylohexane, *in* M-80080
2-(Diethoxymethyl)oxetane, *in* O-80053
2-(Diethoxymethyl)thiazole, *in* T-80170
1,1-Diethoxy-3-nitropropane, *in* N-60037
2,4-Diethoxypyridine, *in* H-60224
2,5-Diethoxypyridine, *in* H-60225
2,6-Diethoxypyridine, *in* H-60226
3,4-Diethoxypyridine, *in* H-60227
2,2-Diethoxytetrahydro-5,6-dimethyl-2*H*-pyran, *in* T-70059
1-[4-[6-(Diethylamino)-2-benzofuranyl]phenyl]-1*H*-pyrrole-2,5-dione, D-60170
2-(Diethylamino)purine, *in* A-60243
2,2-Diethylbutanoic acid, D-60171
Diethyl chlorofumarate, *in* C-80043
Diethyl diacetylfumarate, *in* D-80042
▷ Diethyl dicarbonate, *in* D-70111
Diethyl diethoxymethylmalonate, *in* H-80204
8,14-Diethyl-16,17-dihydro-9,13,24-trimethyl-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[*o*]cyclopent[*b*]azacyclononadecine, *see* E-60042
▷ *N*,*N*′-Diethyl-*N*,*N*′-diphenylurea, *in* D-70499
Diethyl ether 2,2′-dicarboxylic acid, *see* O-80098
▷ Diethylhexyl adipate, *see* B-80148
Di(2-ethylhexyl) sebacate, *see* B-80149
1,2-Diethylidenecyclohexane, D-70154
N,*N*-Diethylnipecotamide, *in* P-70102
N,*N*-Diethyl-3-piperidinecarboxamide, *in* P-70102
1,1-Diethylpropanethiol, *see* E-60053
▷ Diethyl pyrocarbonate, *in* D-70111
Diethyl tartrate, *in* T-70005
▷ *N*,*N*′-Diethylthiocarbamide, *see* D-70155
▷ *N*,*N*′-Diethylthiourea, D-70155
Diethyl(trichlorovinyl)amine, *see* T-70222
1,3-Diethynyladamantane, D-60172
1,8-Diethynylanthracene, D-80155
1,3-Diethynylbenzene, D-70156
1,4-Diethynylbicyclo[2.2.2.]octane, D-70157
2,7-Diethynylnaphthalene, D-70158
1,3-Diethynyl-2,4,5,6-tetrafluorobenzene, D-70159
1,4-Diethynyl-2,3,5,6-tetrafluorobenzene, D-70160
▷ 2,4-Diethynylthiazole, D-80156
▷ 2,5-Diethynylthiophene, D-80157
1,3-Diethynyltricyclo[3.3.1.1^{3,7}]decane, *see* D-60172
Diferuloylmethane, *see* C-80165
▷ Differenol *A*, *see* T-80309
Differentiation inducing factor, *see* T-70335
Diffugenin, *in* D-80350
Diffutidin, *in* T-60103
Diffutin, *in* T-60103
3,3-Difluoroalanine, *see* A-60135
9,10-Difluoroanthracene, D-70161
2,5-Difluorobenzenethiol, D-60173
2,6-Difluorobenzenethiol, D-60174
3,4-Difluorobenzenethiol, D-60175
3,5-Difluorobenzenethiol, D-60176
7,7-Difluorobenzocyclopropene, *see* D-60177
7,7-Difluorobicyclo[4.1.0]hepta-1,3,5-triene, D-60177
4,4′-Difluoro-[1,1′-biphenyl]-3,3′-dicarboxylic acid, D-60178
4,5-Difluoro-[1,1′-biphenyl]-2,3-dicarboxylic acid, D-60179
6,6′-Difluoro-[1,1′-biphenyl]-2,2′-dicarboxylic acid, D-60180
4,4-Difluoro-3,3-bis(trifluoromethyl)-1,2-oxathietane 2,2-dioxide, D-60181
2,2-Difluoro-3,3-bis(trifluoromethyl)oxirane, D-80158
1,1-Difluoro-1,3-butadiene, D-70162
2,2-Difluorobutanedioic acid, D-70163
1,2-Difluoro-2-butenedioic acid, D-80159
2,3-Difluorocinnamaldehyde, *see* D-80164
3,3-Difluorocyclobutanecarboxylic acid, D-70164
3,3-Difluorocyclobutene, D-70165
7,7-Difluorocyclopropabenzene, *see* D-60177
8,8-Difluoro-8,8-dihydro-4-methyl-2,2,6,6-tetrakis(trifluoromethyl)-2*H*,6*H*-[1,2]iodoxolo[4,5,1-*hi*][1,2]benziodoxole, D-60182
3,3-Difluoro-1,2-diiodocyclopropene, D-80160
1,1-Difluoro-2,2-diiodoethylene, D-60183
3,3′-Difluoro-4,4′-dinitrobiphenyl, D-80161
4,4′-Difluoro-2,2′-dinitrobiphenyl, D-80162
5,5′-Difluoro-2,2′-dinitrobiphenyl, D-80163
6,6′-Difluorodiphenic acid, *see* D-60180
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2,2-Difluoroethane *β*-sultone, *see* D-60186
1,2-Difluoroethylene oxide, *see* D-60187
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3,4-Difluoro-2,5-furandione, *in* D-80159
Difluoromaleic acid, *in* D-80159
Difluoromaleic anhydride, *in* D-80159
1,2-Difluoro-4-mercaptobenzene, *see* D-60175
1,3-Difluoro-2-mercaptobenzene, *see* D-60174
1,3-Difluoro-5-mercaptobenzene, *see* D-60176
1,4-Difluoro-2-mercaptobenzene, *see* D-60173
1,1′-(Difluoromethylene)bisbenzene, *see* D-60184
▷ (Difluoromethylene)tetrafluorocyclopropane, D-60185
1,1-Difluoro-10-methyl-3,3,7,7-tetrakis(trifluoromethyl)-4,5,6-benzo-1-ioda-2,8-dioxabicyclo[3.3.0]octane, *see* D-60182
1,3-Difluoro-2-(methylthio)benzene, *in* D-60174
1,3-Difluoro-5-(methylthio)benzene, *in* D-60176
1,4-Difluoro-2-(methylthio)benzene, *in* D-60173
4,4-Difluoro-1,2-oxathietane 2,2-dioxide, D-60186
2,3-Difluorooxirane, D-60187
4,5-Difluorophenanthrene, D-70166
9,10-Difluorophenanthrene, D-70167
2,5-Difluorophenyl mercaptan, *see* D-60173
2,6-Difluorophenyl mercaptan, *see* D-60174
3,4-Difluorophenyl mercaptan, *see* D-60175
3,5-Difluorophenyl mercaptan, *see* D-60176
3,4-Difluoro-6-phenylphthalic acid, *see* D-60179
2,3-Difluoro-3-phenyl-2-propenal, D-80164
2,3-Difluoropyrazine, D-60188
2,6-Difluoropyrazine, D-60189
2,2-Difluorosuccinic acid, *see* D-70163
2,5-Difluorothioanisole, *in* D-60173
2,6-Difluorothioanisole, *in* D-60174

3,5-Difluorothioanisole, *in* D-60176
2,5-Difluorothiophenol, *see* D-60173
2,6-Difluorothiophenol, *see* D-60174
3,4-Difluorothiophenol, *see* D-60175
3,5-Difluorothiophenol, *see* D-60176
Difluoro(trifluoromethanethiolato)(trifluoromethyl)sulfur, *in* T-60281
2,2-Difluoro-3-(trifluoromethyl)-2*H*-azirine, D-80165
2,3-Difluoro-2-(trifluoromethyl)-2*H*-azirine, D-80166
▷ 2,2-Difluorovinyl chloride, *see* C-80049
5-(2,2-Difluorovinyl)-2′-deoxyuridine, *in* D-80167
5-(2,2-Difluorovinyl)uracil, D-80167
Diformylacetic acid, D-60190
3,4-Diformylcinnoline, *see* C-70180
3,5-Diformyl-2,4-dihydroxy-6-methylbenzoic acid 3-hydroxy-4-(methoxycarbonyl)-2,5,6-trimethylphenyl ester, *see* P-70054
3,5-Diformyl-2,4-dihydroxy-6-methylbenzoic acid 3-methoxy-2,5,6-trimethylphenyl ester, *see* N-70032
1,3-Diformylnaphthalene, *see* N-60002
2,9-Diformyl-1,10-phenanthroline, *see* P-80085
1,3-Diformylpyrene, *see* P-80202
3,4-Diformylthiadiazole, *see* T-70162
1,2-Di(2-furanyl)ethylene, D-60191
1,3-Di(2-furyl)benzene, D-70168
1,4-Di(2-furyl)benzene, D-70169
4,6-Di-*O*-galloylarbutin, *in* A-70248
3,5-Digalloylepicatechin, *in* P-70026
▷ Digenic acid, *see* K-60003
▷ Digenin, *see* K-60003
6,8-Di-*C*-glucopyranosylorobol, *see* D-80168
6,8-Di-*C*-glucosyl-3′,4′,5,7-tetrahydroxyisoflavone, D-80168
6,8-Di-*C*-glucosyl-4′,5,7-trihydroxyisoflavone, *see* P-80008
Diglycollic anhydride, *see* D-80500
1,2-Diguaiacyl-1,3-propanediol, *see* B-80150
1,2-Dihydrazinoethane, D-60192
11*β*,13-Dihydro-8-*epi-confertin*, *in* D-60211
2,6-Dihydroaceanthrylene, D-80169
6*b*,7*a*-Dihydroacenaphth[1,2-*b*]oxirene, D-70170
1,2-Dihydro-5-acenaphthylenecarboxylic acid, *see* A-70014
1,2-Dihydro-3,4-acenaphthylenedicarboxylic acid, *see* A-60013
1,2-Dihydro-5,6-acenaphthylenedicarboxylic acid, *see* A-70015
1,2-Dihydro-1-acenaphthylenol, *see* H-80106
1,2-Dihydro-4-acenaphthylenol, *see* H-60099
Dihydroacepentalenediide(2 –), *see* D-60216
9,20-Dihydro-9-(9(10*H*)-acridinylidene)acridine, *see* B-70090
Dihydroaethusanol B, *in* T-80249
Dihydroalterperylenol, *in* A-60078
Dihydroamorphigenin, *in* A-80152
11*β*,13-Dihydroanhydroverlotorin, *in* D-80319
5,10-Dihydroanthra[9,1,2-*cde*]benzo[*rst*]pentaphene, *in* A-60279
9,10-Dihydro-9-anthracenamine, *see* A-60136
9,10-Dihydro-9-anthrylamine, *see* A-60136
11*β*,13-Dihydroartemorin, *in* D-80319
Dihydroatlantonic acid, *in* O-80066
2,3-Dihydro-7-azaindole, *see* D-70263
1,2-Dihydro-3*H*-azepin-3-one, D-70171
2,3-Dihydroazete, D-70172
2,3-Dihydro-6(1*H*)-azulenone, D-60193
9,10-Dihydro-9,10[1′,2′]benzenoanthracene-1,8,13-tricarboxylic acid, *see* T-60399
9,10-Dihydro-9,10[1′,2′]benzenoanthracene-1,8,16-tricarboxylic acid, *see* T-60398
2,3-Dihydro-1*H*-benz[*f*]indene, *see* B-60015
1,2-Dihydrobenz[*f*]isoquinoline, D-80170
3,4-Dihydrobenz[*g*]isoquinoline, D-80171
5,6-Dihydrobenzo[*c*]cinnoline, D-80172
3,4-Dihydro-5,6-benzocoumarin, *see* D-80231
3,4-Dihydro-7,8-benzocoumarin, *see* D-80235
1,4-Dihydrobenzocyclooctatetraene, D-70173
2,3-Dihydro-1*H*-1,4-benzodiazepine, D-80173
2,3-Dihydro-1,4-benzodioxin-2-carboxaldehyde, *see* B-60022
2,3-Dihydro-1,4-benzodioxin-6-carboxaldehyde, *see* B-60023
2,3-Dihydro-1,4-benzodioxin-2-carboxylic acid, *see* B-60024
2,3-Dihydro-1,4-benzodioxin-6-carboxylic acid, *see* B-60025
2,3-Dihydro-1,4-benzodioxin-5,8-dione, D-80174
2,3-Dihydro-1,4-benzodioxin-2-methanol, *see* H-60172
1,8-Dihydrobenzo[2,1-*b*:3,4-*b*′]dipyrrole, D-70174
1,5-Dihydro-2,4-benzodithiepin, D-60194
3,4-Dihydro-2*H*-1,5-benzodithiepin, D-60195
1,4- Dihydro-2,3-benzodithiin, D-80175
2,2′-(4,8-Dihydrobenzo[1,2-*b*:5,4-*b*′]dithiophene-4,8-diylidene)bispropanedinitrile, D-60196
2,3-Dihydro-2-benzofurancarboxylic acid, D-60197
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-2,3,9-triol, *see* T-80335
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,4,9-triol, *see* T-80336
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,9,10-triol, *see* T-80338
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-9-ol, *see* N-80020
3,4-Dihydro-6,7-benzoisocoumarin, *see* D-80237
3,4-Dihydro-7,8-benzoisocoumarin, *see* D-80236
9,18-Dihydrobenzo[*rst*]phenanthro[10,1,2-*cde*]pentaphene, *in* B-60038
3,4-Dihydro-2*H*-1-benzopyran-4-amine, *see* A-80067
3,4-Dihydro-2*H*-1-benzopyran-2-ol, D-60198
3,4-Dihydro-2*H*-1-benzopyran-3-ol, D-60199
3,4-Dihydro-2*H*-1-benzopyran-4-ol, D-60200
3,4-Dihydro-2*H*-1-benzopyran-5-ol, D-60201
3,4-Dihydro-2*H*-1-benzopyran-6-ol, D-70175
3,4-Dihydro-2*H*-1-benzopyran-7-ol, D-60202
3,4-Dihydro-2*H*-1-benzopyran-8-ol, D-60203
1,4-Dihydro-2(3*H*)-benzopyran-3-one, D-70176
1,4-Dihydro-3*H*-2-benzoselenin-3-one, D-60204
3,4-Dihydro-1*H*-2-benzoselenin-3-one, *see* D-60204
1,4-Dihydro-3*H*-2-benzotellurin-3-one, D-60205
3,4-Dihydro-1*H*-2-benzotellurin-3-one, *see* D-60205
3,4-Dihydro-1*H*-2-benzothiin-3-one, *see* D-60206
1,4-Dihydro-3*H*-2-benzothiopyran-3-one, D-60206
1,5-Dihydro-2,3,4-benzotrithiepin, D-80176
3,4-Dihydro-2*H*-1,5-benzoxathiepin-3-one, D-60207
2,3-Dihydro-2′,6″-biluteolin, *in* D-70144
Dihydrobiochanin A, *in* T-80304
2,5-Dihydro-3,5-bis(4-hydroxyphenyl)-2-furanmethanol, *see* C-70201
9,10-Dihydro-9,10-bis(methylene)anthracene, *see* D-70194
1,6-Dihydro-1,6-bis(methylene)azulene, *see* D-60225
2,6-Dihydro-2,6-bis(methylene)azulene, *see* D-60226
1,2-Dihydro-1,2-bis(methylene)naphthalene, *see* D-80187
1,4-Dihydro-1,4-bis(methylene)naphthalene, *see* D-80188
2,3-Dihydro-2,3-bis(methylene)naphthalene, *see* D-80189
2,3-Dihydro-2,3-bis(methylene)thiophene, *see* D-70195
2,3-Dihydro-1,3-bis(phenylmethyl)-1*H*-isoindole, *see* D-80077
11*β*,13-Dihydrobrachynereolide, *in* B-60196
cis-9,10-Dihydrocapsenone, *in* C-60011
1,4-Dihydro-1,4-carbazoledione, *see* C-60012
2,3-Dihydrocarbazol-4(1*H*)-one, *see* O-70106
2,4-Dihydrocarbazol-3(1*H*)-one, *see* O-70105
3,4-Dihydrocarbazol-1(2*H*)-one, *see* O-70103
3,4-Dihydrocarbazol-2(1*H*)-one, *see* O-70104
3,4-Dihydro-*β*-carboline, D-60209
▷ 1*a*,11*c*-Dihydrochryseno[5,6-*b*]oxirene, *see* C-70174
8-Dihydrocinnamoyl-5,7-dihydroxy-4-phenyl-2*H*-benzopyran-2-one, D-60210
Dihydrocochloxanthin, *in* C-60156
Dihydroconfertin, D-60211
11*β*,13-Dihydroconfertin, *in* D-60211
Dihydrocoriandrin, *in* C-70198
Dihydrocumambrin A, *in* C-80164
Dihydrocuneane, *see* T-70022
1,2-Dihydrocyclobuta[*b*]anthracen-1-one, *see* C-80174
4,5-Dihydrocyclobuta[*b*]furan, D-60212
1,2-Dihydrocyclobuta[*a*]naphthalene-2-carboxylic acid, D-70177
1,2-Dihydrocyclobuta[*a*]naphthalene-3,4-dione, D-60213
1,2-Dihydrocyclobuta[*b*]naphthalene-3,8-dione, D-60214
1,2-Dihydrocyclobuta[*a*]naphthalen-3-ol, D-60215
3,8-Dihydrocyclobuta[*b*]quinoxaline-1,2-dione, D-70178
Dihydrocyclopenta[*c,d*]pentalene(2 –), D-60216
2,3-Dihydro-1*H*-cyclopenta[*l*]phenanthrene, D-80177
15,16-Dihydro-17*H*-cyclopenta[*a*]phenanthren-17-one, D-80178
5,6-Dihydro-4*H*-cyclopenta-1,2,3-thiadiazole, D-70179
5,6-Dihydro-4*H*-cyclopentathiophen-4-amine, *see* A-60137
5,6-Dihydro-4*H*-cyclopenta[*b*]thiophene, D-70180
5,6-Dihydro-4*H*-cyclopenta[*c*]thiophene, D-70181
4,5-Dihydro-6*H*-cyclopenta[*b*]thiophen-6-one, D-70182
4,6-Dihydro-5*H*-cyclopenta[*b*]thiophen-5-one, D-70183
5,6-Dihydro-4*H*-cyclopenta[*c*]thiophen-4-one, D-70184
Dihydrodaidzein, *see* D-80322
11*β*,13-Dihydrodesoxoachalensolide, *in* A-70054
1,4-Dihydro-1,4-diazapentalene, *see* D-30286
2,3-Dihydro-2-diazo-3-oxobenzoic acid, *see* D-70063
▷ 10,11-Dihydro-5*H*-dibenz[*b,f*]azepine, D-70185
6,7-Dihydro-5*H*-dibenzo[*a,c*]cycloheptene, D-70186
10,11-Dihydro-5*H*-dibenzo[*a,d*]cycloheptene, D-60217
10,11-Dihydro-5*H*-dibenzo[*a,d*]cyclohepten-5,10-imine, D-80179
5,7-Dihydro-6*H*-dibenzo[*a,c*]cyclohepten-6-one, D-70187
6,7-Dihydro-5*H*-dibenzo[*a,c*]cyclohepten-5-one, D-70188
10,11-Dihydro-5*H*-dibenzo[*a,d*]cyclohepten-5-one, D-60218
5,7-Dihydrodibenzo[*c,e*]selenepin, D-70189
5,7-Dihydrodibenzo[*c,e*]thiepin, D-70190
6,11-Dihydrodibenzo[*b,e*]thiepin-11-one, *see* D-80075
10,11-Dihydrodibenzo[*b,f*]thiepin-10-one, *see* D-80076
1,4-Dihydrodibenzothiophene, D-80180
2,3-Dihydrodicranolomin, *in* D-70144
9,10-Dihydrodicyclopenta[*c*,g]phenanthrene, D-60219
1,10-Dihydrodicyclopenta[*a,h*]naphthalene, D-60220
3,8-Dihydrodicyclopenta[*a,h*]naphthalene, D-60221

1,12-Dihydrodicyclopenta[*c,g*]phenanthrene, *see* D-60219
9,10-Dihydro-5,8:11,14-diethenobenzocyclododecene, *see* B-70038
2,3-Dihydro-2-(1,3-dihydro-1-oxo-2*H*-inden-2-ylidene)-1*H*-inden-1-one, *see* B-80097
2,3-Dihydro-5,7-dihydroxy-3-(2,4-dihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80100
9,10-Dihydro-1,5-dihydroxy-2,7-dimethoxyphenanthrene, *in* T-80114
9,10-Dihydro-1,7-dihydroxy-2,5-dimethoxyphenanthrene, *in* T-80114
9,10-Dihydro-2,7-dihydroxy-3,4-dimethoxyphenanthrene, *in* T-80115
9,10-Dihydro-2,7-dihydroxy-3,5-dimethoxyphenanthrene, *in* T-60120
9,10-Dihydro-5,6-dihydroxy-2,4-dimethoxyphenanthrene, *in* D-70247
9,10-Dihydro-9,10-dihydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *see* K-70013
2,3-Dihydro-5,7-dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, *see* T-80334
1,3-Dihydro-1,4-dihydroxy-5-(hydroxymethyl)-10-methoxy-8-methyl-3,7-dioxo-7*H*-isobenzofuro[4,5-*b*][1,4]benzodioxepin-11-carboxaldehyde, *see* C-60163
3,4-Dihydro-3,4-dihydroxy-2-(hydroxymethyl)-2*H*-pyrrole, D-60222
3,4-Dihydro-6,7-dihydroxy-3-(1-hydroxy-3-oxo-1-butenyl)-4-oxo-2*H*-1-benzopyran-5-carboxylic acid, *see* P-60167
2,3-Dihydro-5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80304
2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-6,8-bis(3-methyl-2-butenyl)-2*H*-1-benzopyran-4-one, *see* S-70034
2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-6,8-bis(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, *see* L-60030
2,3-Dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-2-phenyl-4*H*-1-benzopyran-4-one, *see* G-70015
3,4-Dihydro-5,7-dihydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-benzopyran-6-ylphenylmethanone, *see* B-80056
2,3-Dihydro-3,5-dihydroxy-2-methylnaphthoquinone, D-70191
3,4-Dihydro-4,8-dihydroxy-1(2*H*)-naphthalenone, D-80181
3,4-Dihydro-3-(2,4-dihydroxyphenyl)-6,7-dihydroxy-2*H*-1-benzopyran, *see* T-80098
3,4-Dihydro-2-(3,4-dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran, *see* T-70260
3,4-Dihydro-3-(2,4-dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran, *see* T-80302
2,3-Dihydro-2-(3,4-dihydroxyphenyl)-7-methoxy-3-methyl-5-propenylbenzofuran, *see* K-60001
3′,4′-Dihydro-3′,4′-dihydroxyseselin, *see* K-70013
▷ 2′,3′-Dihydro-3′,6′-dihydroxy-2′,2′,4′,6′-tetramethylspiro[cyclopropane-1,5′-[5*H*]inden]-7′(6′*H*)-one, *see* I-60001
2,3-Dihydro-5,7-dihydroxy-3-(2,3,4-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* P-80039
9,10-Dihydro-2,7-dihydroxy-3,4,6-trimethoxyphenanthrene, *in* D-70246
9,10-Dihydro-5,6-dihydroxy-1,3,4-trimethoxyphenanthrene, *in* P-70034
9,10-Dihydro-6,7-dihydroxy-2,3,4-trimethoxyphenanthrene, *in* D-70246
10,11-Dihydro-5*H*-diindeno[1,2-*b*;2′,1′-*d*]pyrrole, D-80182
10,11-Dihydrodiindeno[1,2-*b*:2′,1′-*d*]thiophene, D-80183
6,11-Dihydro-5*H*-diindolo[2,3-*a*:2′,3′-*c*]carbazole, *see* D-60384
3,8-Dihydro-6,6′;7,3′*a*-diliguetilide, D-60223
2,5-Dihydro-4,6-dimercaptopyrimidine, *see* D-70257
▷ 13,13a-Dihydro-9,10-dimethoxy-3,3-dimethyl-3*H*-bis[1]benzopyrano[3,4-*b*:6′,5′-*e*]pyran-7(7a*H*)one, *see* D-80020
1,2-Dihydro-8,9-dimethoxy-2-(1-methylethenyl)[1]benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(12*H*)one, *see* D-80026
9,10-Dihydro-2,5-dimethoxy-1,7-phenanthrenediol, *in* T-80114
9,10-Dihydro-2,7-dimethoxy-1,5-phenanthrenediol, *in* T-80114
9,10-Dihydro-3,4-dimethoxy-2,7-phenanthrenediol, *in* T-80115
9,10-Dihydro-5,7-dimethoxy-3,4-phenanthrenediol, *in* D-70247
2,5-Dihydro-4,6-dimethoxypyrimidine, *in* D-70256
1,4-Dihydro-3,6-dimethoxy-1,2,4,5-tetrazine, D-70192
9,10-Dihydro-9,9-dimethylanthracene, D-60224
4-[3,4-Dihydro-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-3-yl]-1,3-benzenediol, *see* G-70016
▷ 2,3-Dihydro-2,2-dimethyl-7-benzofuranyl [(dibutylamino)thio]methylcarbamate, *see* C-80022
3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran, D-80184
3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-carboxaldehyde, D-80185
3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-carboxylic acid, D-80186
3-(3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid, *in* D-50601
2,3-Dihydro-2,2-dimethyl-4*H*-1-benzothiopyran, D-70193
9,10-Dihydro-9,10-dimethyleneanthracene, D-70194
1,6-Dihydro-1,6-dimethyleneazulene, D-60225
2,6-Dihydro-2,6-dimethyleneazulene, D-60226
1,2-Dihydro-1,2-dimethylenenaphthalene, D-80187
1,2-Dihydro-1,4-dimethylenenaphthalene, D-80188
2,3-Dihydro-2,3-dimethylenenaphthalene, D-80189
2,3-Dihydro-2,3-dimethylenethiophene, D-70195
2,3-Dihydro-4,5-dimethylfuran, D-80190
Dihydro-4,4-dimethyl-2,3-furandione, D-70196
Dihydro-4,5-dimethyl-2(3*H*)-furanone, D-80191
1,3-Dihydro-1,3-dimethyl-2*H*-imidazo[4,5-*b*]pyrazine-2-thione, *in* D-60247
1,3-Dihydro-1,3-dimethyl-2*H*-imidazo[4,5-*b*]pyrazin-2-one, *in* I-60006
1,4-Dihydro-1,4-dimethyl-2*H*-imidazo[4,5-*b*]pyrazin-2-one, *in* I-60006
2,3-Dihydro-2,2-dimethyl-1*H*-inden-1-one, D-60227
Dihydro-4,4-dimethyl-5-methylene-2(3*H*)-furanone, D-70197
Dihydro-4,5-dimethyl-3-methylene-2(3*H*)-furanone, D-80192
3,4-Dihydro-2,2-dimethyl-1(2*H*)-naphthalenone, D-60228
4,5-Dihydro-4,4-dimethyloxazole, D-70198
2,3-Dihydro-1,6-dimethyl-3-oxopyridazinium hydroxide, inner salt, *in* M-70124
3*a*,6*a*-Dihydro-3*a*,6*a*-dimethyl-1,6-pentalenedione, D-70199
2,3-Dihydro-8,8-dimethyl-2-phenyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, *see* I-80066
2,3-Dihydro-α^2,α^2-dimethyl-6-propyl-2,7-benzofurandimethanol, *see* B-70177
3,7-Dihydro-3,7-dimethyl-6*H*-purin-6-amine, *see* D-60400
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid, D-80193
3,4-Dihydro-2,2-dimethyl-2*H*-pyrrole, D-60229
1,2-Dihydro-2,2-dimethyl-3*H*-pyrrol-3-one, D-60230
3,4-Dihydro-3,3-dimethyl-2(1*H*)quinolinone, D-60231
N-(1,4-Dihydro-1,4-dimethyl-5*H*-tetrazol-5-ylidene)methanamine, *in* A-70202
2,3-Dihydro-2,2-dimethylthiazole, D-80194
2,3-Dihydro-2,2-dimethylthiophene, D-60232
2,3-Dihydro-4,5-dimethylthiophene, D-80195
2,5-Dihydro-2,5-dimethylthiophene, D-60233
4,5-Dihydro-5,5-dimethyl-3*H*-1,2,4-triazol-3-one, D-80196
3,5-Dihydro-4*H*-dinaphth[2,1-*c*:1′,2′-*e*]azepine, D-60234
(6*E*)-10,11-Dihydro-12,19-dioxogeranylnerol, *in* H-60186
6*a*,12*a*-Dihydro-6*H*-[1,3]dioxolo[5,6]benzofuro[3,2-*c*][1]benzopyran-3-ol, *see* M-70001
4,9-Dihydro-4,9-dioxo-1*H*-naphtho[2,3-*d*]-*v*-triazole, *see* N-60011
5,6-Dihydro-11,12-diphenyldibenzo[*a,e*]cyclooctene, D-70202
Dihydro-2,2-diphenyl-2(3*H*)-furanone, D-80197
Dihydro-3,3-diphenyl-2(3*H*)-furanone, D-80198
Dihydro-3,4-diphenyl-2(3*H*)-furanone, D-80199
Dihydro-3,5-diphenyl-2(3*H*)-furanone, D-80200
Dihydro-4,4-diphenyl-2(3*H*)-furanone, D-80201
Dihydro-4,5-diphenyl-2(3*H*)-furanone, D-80202
Dihydro-5,5-diphenyl-2(3*H*)-furanone, D-80203
▷ 2,3-Dihydro-5,6-diphenyl-1,4-oxathiin, D-70203
1,2-Dihydro-4,6-diphenylpyrimidine, D-60235
2,5-Dihydro-3,6-diphenylpyrrolo[3,4-*c*]pyrrole-1,4-dione, D-70204
2,5-Dihydro-3,4-diphenylselenophene, D-70205
2,5-Dihydro-2,2-diphenyl-1,3,4-thiadiazole, D-60236
2,5-Dihydro-1*H*-dipyrido[4,3-*b*:3′,4′-*d*]pyrrol-1-one, D-60237
5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-one, D-80205
5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-thione, D-80206
2-(5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-ylidene)-5,6-dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin, D-60238
Dihydrodroserone, *see* D-70191
7,7-*O*-Dihydroebuloside, *in* E-60001
β-Dihydroentandrophragmin, *in* E-70009
9,10-Dihydro-9,10-epidithioanthracene, D-70206
11β,13-Dihydroepiligustrin (incorr.), *in* D-60328
5,6-Dihydroergosterol, *in* M-80059
11α,13-Dihydroestafialin, *in* E-80057
9,10-Dihydro-9,10-ethanoanthracene, D-70207
4,5-Dihydro-1,5-ethano-1*H*-1-benzazepin-2(3*H*)-one, D-60239
4,7-Dihydro-4,7-ethanoisobenzofuran, D-60240
1,4-Dihydro-1,4-ethanonaphtho[1,8-*de*][1,2]diazepine, D-80207
9,10-Dihydro-9,10-ethenoanthracene-11,12-dicarboxylic acid, D-70208
5,6-Dihydro-2-(ethylthio)-4*H*-1,3-thiazine, *in* T-60094

3,4-Dihydro-3-fluoro-2*H*-1,5-benzodioxepin, D-70209
Dihydro-3-fluoro-2(3*H*)-furanone, D-80208
Dihydroformononetin, *in* D-80322
Dihydrofumigatin, *in* M-80050
Dihydro-2,3(2*H*,3*H*)-furandione, *in* H-80227
Dihydro-2(3*H*)-furanthione, D-70210
1-(4,5-Dihydro-3-furanyl)-2,2,2-trifluoroethanone, *see* D-70274
1,4-Dihydrofuro[3,4-*d*]pyridazine, D-60241
2,3-Dihydrofuro[2,3-*b*]pyridine, D-70211
Dihydrofusarubin *A*, *in* F-60108
Dihydrofusarubin *B*, *in* F-60108
▷ 1,2-Dihydrogedunin, *in* G-70006
5α,6-Dihydroglaucasterol, *in* P-60004
9,11-Dihydrogracilin *A*, *in* G-60033
Dihydroguaiaretic acid, *in* G-70033
2,3-Dihydro-3′,4′,4″,5,5″,7,7″-heptahydroxy-3,8′-biflavone, D-80209
10,15-Dihydro-2,3,7,8,12,13-hexamethoxy-5*H*-tribenzo[*a*,*d*,*g*]cyclononene, *see* C-70254
3,8-Dihydro-3,3,4,8,8,9-hexamethylbenzo[1,2-*c*:4,5-*c*′]dipyran-1,6-dione, *see* T-70190
2,3-Dihydro-1,1,2,2,3,3-hexamethyl-1*H*-indene, *see* H-80075
Dihydro-3,3,4,4,5,5-hexamethyl-2*H*-pyran-2,6(3*H*)-dione, D-80210
Dihydro-3,3,4,4,5,5-hexamethyl-2*H*-pyran-2,6(3*H*)dione, *in* H-80076
Dihydrohomalicine, *in* H-70207
2,3-Dihydro-2-hydroxybenzo[*b*]furan-3-one, *see* H-80107
4-(3,4-Dihydro-7-hydroxy-2*H*-1-benzopyran-4-yl)-1,3-benzenediol, *see* T-80302
5-(3,4-Dihydro-7-hydroxy-2*H*-1-benzopyran-3-yl)-2,3-dimethoxy-2,5-cyclohexadiene-1,4-dione, *see* P-80018
4-(3,4-Dihydro-7-hydroxy-2*H*-1-benzopyran-3-yl)-6-(1,1-dimethyl-2-propenyl)-3-methoxy-1,2-benzenediol, *in* U-80002
10,11-Dihydro-11-hydroxycurcuphenol, *in* C-70208
2,3-Dihydro-7-hydroxy-3-(2,4-dihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80303
13,13*a*-Dihydro-7*a*-hydroxy-9,10-dimethoxy-3,3-dimethyl-3*H*-bis[1]benzopyrano[3,4-*b*:6′,5′-*e*]pyran-7(7*aH*)-one, *see* T-80009
13,13*a*-Dihydro-6-hydroxy-9,10-dimethoxy-3,3-dimethyl-3*H*-bis[1]benzopyrano[3,4-*b*:6′,5′-*e*]pyran-7(7*aH*)-one, *see* T-80204
2,3-Dihydro-10-hydroxy-3,3-dimethyl-1*H*,7*H*-furo[2,3-*c*:5,4-*f*′]bis[1]benzopyran-7-one, *see* S-80037
Dihydro-3-hydroxy-2,5-furandione, D-80211
Dihydro-3-hydroxy-2(3*H*)-furanone, D-80212
Dihydro-4-hydroxy-2(3*H*)-furanone, D-60242
4,5-Dihydro-3-hydroxy-2(3*H*)-furanone, *in* D-60313
3*a*,7*a*-Dihydro-4-hydroxy-4*H*-furo[2,3-*b*]pyran-2(3*H*)-one, *see* O-70107
11β,13-Dihydro-8α-hydroxyglucozaluzanin *C*, *in* Z-60001
7,8-Dihydro-12β-hydroxyholothurinogenin, *in* T-70267
2,3-Dihydro-7-hydroxy-2-[4-hydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, *see* A-80009
2,3-Dihydro-7-hydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one,9CI, *see* A-80007
2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-6-(4-hydroxyphenyl)-5*H*-furo[3,2-*g*][1]benzopyran-5-one, *see* E-80054
4,5-Dihydro-3-hydroxy-5-(hydroxymethyl)-2(3*H*)-furanone, D-70212
2,3-Dihydro-7-hydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* D-80322
2,3-Dihydro-7-hydroxy-3-[(4-hydroxyphenyl)methylene]-4*H*-1-benzopyran-4-one, *see* H-60152
2,3-Dihydro-2-hydroxy-1*H*-imidazole-4,5-dione, D-60243
3,4-Dihydro-11-hydroxy-5-methoxy-2,2-dimethyl-2*H*,8*H*-benzofuro[3,2-*c*]pyrano[2,3-*f*][1]benzopyran-8-one, *see* I-80061
3,4-Dihydro-4-hydroxy-6-methoxy-2,7-dimethyl-1(2*H*)-naphthalenone, *see* F-60014
2,3-Dihydro-5-hydroxy-8-methoxy-2,4-dimethylnaphtho[1,2-b]furan-6,9-dione, D-80213
1,3,Dihydro-8-hydroxy-5-methoxy-6,7-methylenedioxy-1-methylnaphtho[2,3-*c*]furan-4,9-dione, *see* V-60004
2,3-Dihydro-2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-3-methylbenzofuran, *in* D-60244
2,3-Dihydro-7-hydroxy-3-[4-methoxyphenyl)methylene]-4*H*-1-benzopyran-4-one, *see* B-60192
2,3-Dihydro-2-(4-hydroxy-3-methoxyphenyl)-3-methyl-5-(1-propenyl)benzofuran, *in* C-60161
3,4-Dihydro-8-hydroxy-3-methylbenz[*a*]anthracene-1,7,12(2*H*)-trione, *see* O-60003
2,3-Dihydro-3-hydroxy-2-(1-methylethenyl)-5-benzofurancarboxaldehyde, D-70213
1-[2,3-Dihydro-5-hydroxy-2-(1-methylethenyl)-4-benzofuranyl]ethanone, *see* A-70040
2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-5-benzofurancarboxaldehyde, D-70214
Dihydro-4-hydroxy-3-methyl-2(3*H*)-furanone, D-80214
Dihydro-4-hydroxy-5-methyl-2(3*H*)furanone, *in* D-80353
2,3-Dihydro-7-hydroxymethyl-2-(2-hydroxy-2-propyl)-6-propylbenzofuran, *see* B-70177
7,12-Dihydro-11-hydroxy-2-(1-methylpropyl)-4,7,12-trioxo-4*H*-anthra[1,2-*b*]pyran-5-acetic acid, *see* A-70239
1,3-Dihydro-1-hydroxynaphtho[2,3-*c*]furan, *see* H-60188
4,5-Dihydro-6-hydroxy-3-oxo-8′-apo-ε-caroten-8′-oic acid, *in* C-60156
▷ 1,3-Dihydro-1-hydroxy-3-oxo-1,2-benziodoxole, *see* H-60102
3,4-Dihydro-3-(3-hydroxyphenyl)-1*H*-2-benzopyran-1-one, *in* H-70207
3,4-Dihydro-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-3,5,7-triol, *see* T-60104
2,3-Dihydro-2-(4-hydroxyphenyl)-5-(3-hydroxypropyl)-3-methylbenzofuran, D-60244
2,3-Dihydro-2-(4-hydroxyphenyl)-7-methoxy-3-methyl-5-(1-propenyl)benzofuran, *in* C-60161
2,3-Dihydro-2-(4-hydroxyphenyl)-3-methyl-5-benzofuranpropanol, *see* D-60244
2,3-Dihydro-2-(4-hydroxyphenyl)-3-methyl-5-(1-propenyl)benzofuran, *see* C-60161
1,2-Dihydro-5-hydroxy-4-phenyl-3*H*-pyrazol-3-one, *see* D-80369
22,23-Dihydro-24-hydroxyrotenone, *in* A-80152
6′,7′-Dihydro-6′-hydroxyrotenone, *see* D-80003
9,10-Dihydro-7-hydroxy-2,3,4,6-tetramethoxyphenanthrene, *in* D-70246
3,4-Dihydro-7-hydroxy-3-(2,3,4-trihydroxyphenyl)-2*H*-1-benzopyran, *see* T-80095
3,4-Dihydro-7-hydroxy-3-(2,4,5-trihydroxyphenyl)-2*H*-1-benzopyran, *see* T-80097
2,3-Dihydro-7-hydroxy-3-(2,3,4-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80099
11β,13-Dihydro-9α-hydroxyzaluzanin*C*, *in* Z-60001
4,5-Dihydro-1*H*-imidazole, D-60245
1,3-Dihydro-2*H*-imidazole-2-thione, D-80215
1-(4,5-Dihydro-1*H*-imidazol-2-yl)-2-imidazolidinethione, D-60246
1,3-Dihydro-2*H*-imidazo[4,5-*b*]pyrazine-2-thione, D-60247
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazine-6-thione, D-70215
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazin-6-one, D-60248
2,3-Dihydroimidazo[1,2-*a*]pyridine, D-70216
1,3-Dihydro-2*H*-imidazo[4,5-*b*]pyridin-2-one, D-60249
1,3-Dihydro-2*H*-imidazo[4,5-*c*]pyridin-2-one, D-60250
1,5-Dihydro-8*H*-imidazo[4,5-*g*]quinazolin-8-one, I-60012
1,4-Dihydro-5-imino-3,4-dimethyltetrazole, *in* A-70202
4,5-Dihydro-5-imino-*N*,4-diphenyl-1,2,4-thiadiazol-3-amine, *see* H-60012
5,6-Dihydro-4*H*-indene, D-70217
1,3-Dihydro-1,1,3,3-2*H*-indene-2-selone, *see* T-60142
5,10-Dihydroindeno[2,1-*a*]indene, D-70218
4*b*,9*a*-Dihydroindeno[1,2-*a*]indene-9,10-dione, D-70219
4*b*,9*b*-Dihydroindeno[2,1-*a*]indene-5,10-dione, D-70220
5,10-Dihydroindeno[1,2-*b*]indole, D-80216
1-(2,3-Dihydro-1*H*-inden-1-ylidene)-2,3-dihydro-1*H*-indene, *see* B-70120
2,3-Dihydro-1*H*-indole-2-sulfonic acid, D-70221
2,3-Dihydro-5(1*H*)-indolizinone, D-60251
11β,13-Dihydro-1-*epi*-inuviscolide, *in* I-70023
11α,13-Dihydroinuviscolide, *in* I-70023
11β,13-Dihydroinuviscolide, *in* I-70023
Dihydro-3-iodo-2(3*H*)-furanone, D-60252
Dihydroiresin, *in* I-80043
Dihydroiresone, *in* I-80043
Dihydroisoalantolactone, *in* I-80046
4,7-Dihydroisobenzofuran, D-60253
1,3-Dihydro-1-isobenzofuranol, *see* H-60171
2,3-Dihydro-1*H*-isoindol-1-one, *see* P-70100
3,4-Dihydro-8-isopropyl-5-methyl-2-naphthalenecarboxaldehyde, *in* I-60129
2,3-Dihydro-1,4-isoquinolinedione, D-80217
7,8-Dihydro-5(6*H*)-isoquinolinone, D-60254
9,10-Dihydrojasmonic acid, *see* O-80091
11,12-Dihydrolinderazulene, *in* L-70031
2,3-Dihydrolinderazulene, *in* L-70031
Dihydrolippione, *in* P-80153
Dihydromaackiain, *in* T-80097
Dihydromatricaria acid, *see* D-70018
7,12-Dihydro-5*H*-6,12-methanodibenz[*c*,*f*]azocine, D-60255
1,4-Dihydro-1,4-methanonaphthalene, D-60256
2,3-Dihydro-1,2,3-metheno-1*H*-indene, *see* N-60012
5,6-Dihydro-4,5,6-metheno-4*H*-indene, *see* T-70019
2,3-Dihydro-1,2,3-metheno-1*H*-phenalene, D-80218
3,4-Dihydro-6-methoxy-2*H*-1-benzopyran, *in* D-70175
3,4-Dihydro-8-methoxy-2*H*-1-benzopyran, *in* D-60203
3,4-Dihydro-5-methoxy-8,8-dimethyl-2-phenyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-ol, *see* T-70007
6*a*,13*a*-Dihydro-8-methoxy-1,3-dioxolo[6,7][1]benzopyrano[3,4-*b*]furo[3,2-*g*]benzopyran-13(16*H*)-one, *see* P-80004
Dihydro-3-methoxy-2,5-furandione, *in* D-80211
4,5-Dihydro-3-(methoxymethylene)-2(3*H*)-furanone, D-70222
8,9-Dihydro-5-methoxy-8-(1-methylethenyl)-2-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran, *see* A-70002
8,8*a*-Dihydro-3-methoxy-5-methyl-1*H*,6*H*-furo[3,4-*e*][1,3,2]dioxaphosphepin 3-oxide, D-70223

2,3-Dihydro-7-methoxy-3-methyl-5-(1-propenyl)-2-(3,4,5-trimethoxyphenyl)benzofuran, *see* L-60024
15,16-Dihydro-15-methoxy-16-oxohardwickiic acid, *in* H-70002
15,16-Dihydro-15-methoxy-16-oxonidoresedic acid, *in* N-70035
3,4-Dihydro-5-methoxy-4-oxo-2-(1-pentenyl)-2*H*-1-benzopyran-7-acetic acid, *see* C-60025
15,16-Dihydro-15-methoxy-16-oxostrictic acid, *in* S-70077
9,10-Dihydro-4-methoxy-2,7-phenanthrenediol, *in* P-80080
9,10-Dihydro-7-methoxy-2,5-phenanthrenediol, *in* P-80080
3,4-Dihydro-5-methoxy-2*H*-pyrrole, *in* P-70188
▷ 1,2-Dihydro-6-methylbenz[*j*]aceanthrylene, *see* M-70056
6*a*,11*a*-Dihydro-10-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,9-diol, *see* P-80076
10,11-Dihydro-5-methyl-5*H*-dibenz[*b*,*f*]azepine, *in* D-70185
10,11-Dihydro-5-methylene-5*H*-dibenzo[*a*,*d*]cycloheptene, D-80219
2,3-Dihydro-1-methylene-1*H*-indene, *see* M-60078
3,4-Dihydro-1(2*H*)-methylenenaphthalene, *see* T-60073
Dihydro-3-methylene-4-octylfuro[3,4-*b*]furan-2,6(3*H*,4*H*)-dione, *see* A-60325
1-[2,3-Dihydro-2-(1-methylethenyl)-5-benzofuranyl]-1,2-propanediol, *see* D-70340
1,3-Dihydro-3-(1-methylethyl)-2*H*-indol-2-one, *see* I-70097
Dihydro-4-methyl-2(3*H*)-furanone, D-80220
5-(7,10-Dihydro-8-methylfuro[2,3-*g*][1]benzoxepin-2-yl)-1,3-benzenediol, *see* M-60145
1,3-Dihydro-1-methyl-2*H*-imidazo[4,5-*b*]pyrazine-2-thione, *in* D-60247
1,3-Dihydro-1-methyl-2*H*-imidazo[4,5-*b*]pyrazin-2-one, *in* I-60006
Dihydro-4-methyl-5-(3-methyl-2-butenyl)-2(3*H*)-furanone, *see* E-70004
Dihydro-4-methyl-3-methylene-2(3*H*)-furanone, D-80222
1,2-Dihydro-1-methyl-2-oxoadenosine, *see* D-60518
7-[[4-(2,5-Dihydro-4-methyl-5-oxo-2-furanyl)-3-methyl-2-butenyl]oxy]-2*H*-1-benzopyran-2-one, D-80223
7-[[3-[(2,5-Dihydro-4-methyl-5-oxo-2-furanyl)methyl]-3-methyloxiranyl]methoxy]-2*H*-1-benzopyran-2-one, *in* D-80223
4-(1,5-Dihydro-3-methyl-5-oxo-1-phenyl-4*H*-pyrazol-4-ylidene)-2,4-dihydro-5-methyl-2-phenyl-3*H*-pyrazol-3-one, *see* P-70153
N-(2,9-Dihydro-1-methyl-2-oxo-1*H*-purin-6-yl)acetamide, *in* A-60144
1,4-Dihydro-6-methyl-4-oxo-3-pyridinecarboxylic acid, D-80224
1,6-Dihydro-3-methyl-6-oxo-2-pyridinecarboxylic acid, D-80225
1,6-Dihydro-5-methyl-6-oxo-2-pyridinecarboxylic acid, D-80226
Dihydro-4-methyl-5-pentyl-2(3*H*)-furanone, D-80227
4-[2,3-Dihydro-3-methyl-5-(1-propenyl)-2-benzofuranyl]phenol, *see* C-60161
4,5-Dihydro-2-(1-methylpropyl)thiazole, D-70224
3,9-Dihydro-9-methyl-1*H*-purine-2,6-dione, D-60257
5,6-Dihydro-3-methyl-2*H*-pyran-2-one, D-80228
5,6-Dihydro-4-methyl-2*H*-pyran-2-one, *in* H-80211
3,4-Dihydro-6-methyl-2(1*H*)-pyridinone, D-80229
1,4-Dihydro-2-methylpyrimidine, D-70225
1,6-Dihydro-2-methylpyrimidine, *see* D-70225
3,4-Dihydro-5-methyl-2*H*-pyrrole, D-70226
2,3-Dihydro-2-methylthiophene, D-70227
2,3-Dihydro-4-methylthiophene, D-70228
2,3-Dihydro-5-methylthiophene, D-70229
2,5-Dihydro-2-methylthiophene, D-70230
2,5-Dihydro-3-methylthiophene, D-70231
5,6-Dihydro-2-(methylthio)-4*H*-1,3-thiazine, *in* T-60094
4,5-Dihydro-2-(methylthio)thiazole, *in* T-60197
3,4-Dihydro-5-methyl-4-thioxo-2(1*H*)-pyrimidinone, D-70233
3,4-Dihydro-6-methyl-4-thioxo-2(1*H*)-pyrimidinone, D-70234
10,11-Dihydromicroglossic acid, *in* M-60134
Dihydromyoporone, *in* M-60156
Dihydro-5-myristoyl-2(3*H*)-furanone, *see* F-80004
1,4-Dihydro-1-naphthalenamine, *see* A-60139
5,8-Dihydro-1-naphthalenamine, *see* A-60140
1-(3,4-Dihydro-1(2*H*)-naphthalenylidene)-1,2,3,4-tetrahydronaphthalene, *see* B-70165
2,3-Dihydronaphtho[2,3-*b*]furan, D-70235
2*H*-3,4-Dihydronaphtho[2,3-*b*]pyran-5,10-dione, D-80230
1,2-Dihydro-3*H*-naphtho[2,1-*b*]pyran-3-one, D-80231
2,3-Dihydro-1*H*-naphtho[2,1-*b*]pyran-1-one, D-80232
2,3-Dihydro-4*H*-naphtho[1,2-*b*]pyran-4-one, D-80233
2,3-Dihydro-4*H*-naphtho[2,3-*b*]pyran-4-one, D-80234
3,4-Dihydro-2*H*-naphtho[1,2-*b*]pyran-2-one, D-80235
3,4-Dihydro-1*H*-naphtho[1,2-*c*]pyran-3-one, D-80236
3,4-Dihydro-1*H*-naphtho[2,3-*c*]pyran-1-one, D-80237
1*a*,7*a*-Dihydronaphth[2,3-*b*]oxirene-2,7-dione, *see* E-70011
1,4-Dihydro-1-naphthylamine, *see* A-60139
5,8-Dihydro-1-naphthylamine, *see* A-60140
Dihydronarigenin, *see* H-80244
Dihydroniloticin, *in* N-70036
2,3-Dihydro-4-nitro-2,3-dioxo-9,10-secostrychnidin-10-oic acid, *see* C-70001
2,5-Dihydro-3-nitrofuran, D-70236
2,5-Dihydro-2-(4,6,8-nonatrien-2-ynylidene)furan, D-80238
11-Dihydro-12-norneoquassin, D-60258
2,3-Dihydroononin, *in* D-80322
9,11-Dihydro-22,25-oxido-11-oxoholothurinogenin, D-70237
3,4-Dihydro-3-oxo-2*H*-1,4-benzothiazine, *see* B-80043
3,4-Dihydro-4-oxo-1,2,3-benzothiazine, *see* B-80052
7,8-Dihydro-8-oxoguanosine, D-70238
15,16-Dihydro-16-oxohardwickiic acid, *in* H-70002
2,3-Dihydro-2-oxo-1*H*-indole-3-acetic acid, D-60259
(1,2-Dihydro-2-oxo-3*H*-indol-3-ylidene)hydroxyacetic acid, *see* O-80085
4,5-Dihydro-2-oxo-3*H*-oxazole-4-carboxylic acid, *see* O-60082
3,4-Dihydro-4-oxopyrido[2,3-*d*]pyrimidine-2(1*H*)-thione, *see* D-60291
5,6-Dihydro-4-oxopyrimidine, *see* D-60274
N-(1,4-Dihydro-4-oxo-5-pyrimidinyl)formamide, *in* A-70196
2,3-Dihydro-3-oxo-1*H*-pyrrole-1-carboxaldehyde, *in* D-70262
4,5-Dihydro-5-(1-oxotetradecyl)-2(3*H*)furanone, *see* F-80004
Dihydropallescensin 2, *see* P-60015
Dihydropanaxacol, *in* D-80321
Dihydroparthenin, *in* P-80011
Dihydroparthenolide, D-70239
9,10-Dihydropentafulvalene, *see* B-60100
9,10-Dihydro-2,3,4,6,7-pentahydroxyphenanthrene, *see* D-70246
1,2-Dihydropentalene, D-70240
1,4-Dihydropentalene, D-70241
1,5-Dihydropentalene, D-70242
1,6-Dihydropentalene, D-70243
1,6*a*-Dihydropentalene, D-70244
▷ Dihydro-5-pentyl-2(3*H*)-furanone, D-70245
2,2-Dihydroperfluoropropane, *see* H-80050
9,10-Dihydro-2-phenanthrenamine, *see* A-60141
9,10-Dihydro-4-phenanthrenamine, *see* A-60142
9,10-Dihydro-9-phenanthrenamine, *see* A-60143
9,10-Dihydrophenanthrene, D-60260
9,10-Dihydro-2,3,4,6,7-phenanthrenepentol, D-70246
9,10-Dihydro-2,4,5,6-phenanthrenetetrol, D-70247
9,10-Dihydro-2-phenanthrylamine, *see* A-60141
9,10-Dihydro-4-phenanthrylamine, *see* A-60142
9,10-Dihydro-9-phenanthrylamine, *see* A-60143
2,3-Dihydro-2-phenyl-1,2-benzisothiazole, D-60261
2,3-Dihydro-2-phenyl-2-benzofurancarboxylic acid, D-60262
2,3-Dihydro-2-phenyl-4*H*-benzo[*b*]thiin-4-one, *see* D-70248
2,3-Dihydro-2-phenyl-4*H*-1-benzothiopyran-4-one, D-70248
10,11-Dihydro-5-phenyl-5*H*-dibenz[*b*,*f*]azepine, *in* D-70185
▷ 5,6-Dihydro-6-(2-phenylethenyl)-2*H*-pyran-2-one, *see* G-60031
Dihydro-5-phenyl-2(3*H*)-furanone, D-80239
2,3-Dihydro-3-(phenylmethylene)-4*H*-1-benzopyran-4-one, D-60263
1,2-Dihydro-1-phenyl-1-naphthalenecarboxylic acid, D-60264
3,4-Dihydro-2-phenyl-1(2*H*)-naphthalenone, D-60265
3,4-Dihydro-3-phenyl-1(2*H*)-naphthalenone, D-60266
3,4-Dihydro-4-phenyl-1(2*H*)-naphthalenone, D-60267
1,2-Dihydro-1-phenyl-1-naphthoic acid, *see* D-60264
1,4-Dihydro-2-phenylpyrimidine, D-70249
1,6-Dihydro-2-phenylpyrimidine, *see* D-70249
5,6-Dihydro-6-phenyl-2,4(1*H*, 3*H*)-pyrimidinedione, D-80240
5,6-Dihydro-2-phenyl-4(1*H*)-pyrimidinone, D-70250
4,5-Dihydro-2-phenyl-6(1*H*)-pyrimidinone, *see* D-70250
3,4-Dihydro-5-phenyl-2*H*-pyrrole, D-70251
1,2-Dihydro-1-phenyl-3*H*-pyrrol-3-one, *in* D-70262
2,3-Dihydro-6-phenyl-2-thioxo-4(1*H*)-pyrimidinone, D-60268
1,2-Dihydro-5-phenyl-3*H*-1,2,4-triazol-3-one, D-80241
Dihydropinosylvin, *see* P-80100
Dihydropinosylvin methyl ether, *in* P-80100
7,12-Dihydropleiadene, D-60269
Dihydroplexaurolone, *in* P-80163
11,13-Dihydropsilostachyin, *in* P-70131
1,5-Dihydro-2,4,6(3*H*)-pteridinetrione, *see* P-70134
▷ 1,7-Dihydro-6*H*-purine-6-thione, D-60270
3,4-Dihydro-2*H*-pyran-5-carboxaldehyde, D-70252
3,6-Dihydro-2*H*-pyran-2-carboxylic acid, D-80242
3,6-Dihydro-2*H*-pyran-2,2-dicarboxylic acid, D-80243
3,4-Dihydro-2*H*-pyrano[2,3-*b*]pyridine, D-80244

1-(3,4-Dihydro-2*H*-pyran-5-yl)-2,2,2-trifluoroethanone, *see* D-70275
4,5-Dihydro-1*H*-pyrazole, D-70253
1,8-Dihydro-5*H*-pyrazolo[4,3-*g*]quinazolin-5,7(6*H*)-dione, *see* P-60203
3,8-Dihydro-9*H*-pyrazolo[4,3-*f*]quinazolin-9-one, D-60271
1,6-Dihydro-5*H*-pyrazolo[4,3-*g*]quinazolin-5-one, *see* P-60205
3,5-Dihydro-4*H*-pyrazolo[3,4-*c*]quinolin-4-one, D-80245
1,2-Dihydro-3,6-pyridazinedithione, *see* M-80028
4,5-Dihydro-3(2*H*)-pyridazinone, D-60272
7,12-Dihydropyrido[3,2-*b*:5,4-*b*′]diindole, D-70254
7,12-Dihydropyrido[3,2-*b*:5,4-*b*′]diindole, D-80246
4,9-Dihydro-3*H*-pyrido[3,4-*b*]indole, *see* D-60209
1,4-Dihydropyrimidine, D-70255
1,6-Dihydropyrimidine, *see* D-70255
Dihydropyrimidine, *see* D-70255
2,5-Dihydro-4,6-pyrimidinediol, *see* D-70256
Dihydro-4,6-(1*H*,5*H*)-pyrimidinedione, D-70256
2,5-Dihydro-4,6-pyrimidinedithiol, D-70257
3,4-Dihydro-2(1*H*)-pyrimidinone, D-60273
5,6-Dihydro-4(1*H*)-pyrimidinone, D-60274
6,7-Dihydro-5*H*-1-pyrindine, D-60275
6,7-Dihydro-5*H*-2-pyrindine, D-60276
3,4-Dihydro-2*H*-pyrrole, D-80247
3,4-Dihydro-2*H*-pyrrole-2-carboxylic acid, D-80248
3,4-Dihydro-2*H*-pyrrole-5-carboxylic acid, D-80249
Dihydro-1*H*-pyrrolizine-3,5(2*H*,6*H*)-dione, D-70260
2,3-Dihydro-1*H*-pyrrolizin-1-ol, D-70261
2,3-Dihydro-1*H*-pyrrolizin-1-one, D-60277
2,3-Dihydro-1*H*-pyrrolizin-6(5*H*)-one, D-80250
2,5-Dihydro-1*H*-pyrrolo[3,2-*c*:4,5-*c*′]dipyridin-1-one, *see* D-60237
1,2-Dihydro-3*H*-pyrrol-3-one, D-70262
2,3-Dihydro-1*H*-pyrrolo[2,3-*b*]pyridine, D-70263
2,3-Dihydro-1*H*-pyrrolo[3,2-*c*] pyridine, D-80251
1,6-Dihydro-7*H*-pyrrolo[2,3-*c*]pyridin-7-one, D-80252
1,4-Dihydropyrrolo[3,2-*b*]pyrrole, D-30286
▷ Dihydroquercetin, *see* P-70027
3,4-Dihydro-2(1*H*)-quinazolinone, D-60278
5,12-Dihydroquino[2,3-*b*]acridine-7,14-dione, *see* Q-80001
5,7-Dihydroquino[3,2-*b*]acridine-12,14-dione, *see* I-80086
1,4-Dihydro-2,3-quinoxalinedione, D-60279
5,14-Dihydroquinoxalino[2,3-*b*]phenazine, D-70264
Dihydrorecifeiolide, *in* H-80157
Dihydroridentin, *in* R-70007
7-Dihydrosamaderine B, *in* S-80007
7-Dihydrosamaderine C, *in* S-80007
Dihydrosamidin, *in* K-70013
2,3-Dihydro-2-selenoxo-4(1*H*)-quinazolinone, D-60281
3,4-Dihydro-4-selenoxo-2(1*H*)-quinazolinone, D-60280
Dihydroserruloside, D-70265
Dihydrosinapic aldehyde, *in* T-80333
▷ 5,6-Dihydro-6-styryl-2-pyranone, *see* G-60031
Dihydrosuberenol, *in* S-70080
6*a*,12*a*-Dihydro-2,3,8,10-tetrahydroxy[2]benzopyrano[4,3-*b*][1]benzopyran-7(5*H*)-one, *see* C-70200
10,11-Dihydro-2,4,7,8-tetrahydroxy-10-(3,4-dihydroxyphenyl)-5-[(3,5-dihydroxyphenyl)methyl]-5*H*-dibenzo[*a*,*d*]cycloheptene, *see* C-70025
5,6-Dihydro-6-(2,4,6,10-tetrahydroxyheneicosyl)-2*H*-pyran-2-one, *in* D-70276
9,10-Dihydro-3,4,6,7-tetramethoxy-2-phenanthrenol, *in* D-70246
4,7-Dihydro-1,1,3,3-tetramethyl-1*H*,3*H*-3*a*,7*a*-episeleno-4,7-epoxyisobenzofuran, D-70266
Dihydro-3,3,4,4-tetramethyl-2(3*H*)-furanthione, D-60282
17,17*a*-Dihydro-4,4,8,17-tetramethyl-3′*H*-indeno[1′,2′:17,17*a*]-D-homoandrost-17-ene-4′,6′,7′-triol, *see* D-60499
1,3-Dihydro-1,1,3,3-tetramethyl-2*H*-inden-2-one, *see* T-60143
4,5-Dihydro-3,3,5,5-tetramethyl-4-methylene-3*H*-pyrazole, D-60283
3,4-Dihydro-3,3,6,8-tetramethyl-1(2*H*)-napthalenone, D-80254
2,5-Dihydro-2,2,5,5-tetramethyl-3-[[[(2-phenyl-3*H*-indol-3-ylidene)amino]oxy]carbonyl]-1*H*-pyrrol-1-yloxy, D-60284
3,5-Dihydro-3,3,5,5-tetramethyl-4*H*-pyrazole-4-thione, D-60285
3,5-Dihydro-3,3,5,5-tetramethyl-4*H*-pyrazol-4-one, D-60286
3,6-Dihydro-3,3,6,6-tetramethyl-2(1*H*)-pyridinone, D-70267
4,5-Dihydro-3,3,4,4-tetramethyl-2(3*H*)-thiophenethione, D-60287
4,5-Dihydro-3,3,4,4-tetramethyl-2(3*H*)-thiophenone, D-60288
3,4-Dihydro-3,3,4,4-tetramethyl-5-thioxo-2(1*H*)pyrrolidinone, D-80255
1,2-Dihydro-1,2,4,5-tetrazine-3,6-dione, D-70268
1,4-Dihydro-5*H*-tetrazole-5-thione, *see* T-60174
1,4-Dihydro-5*H*-tetrazol-5-one, *see* T-60175
7,8-Dihydrotetrazolo[1,5-*b*][1,2,4]triazine, D-80256
1,7-Dihydrotetrazolo[1,5-*b*][1,2,4]triazine, *see* D-80256
1-(4,5-Dihydro-2-thiazolyl)ethanone, *see* A-70041
1,4-Dihydrothieno[3,4-*d*]pyridazine, D-60289
2,3-Dihydrothieno[2,3-*b*]pyridine, D-70269
6,7-Dihydro-5*H*-thieno[3,2-*b*]thiopyran, D-80257
6,7-Dihydro-4*H*-thieno[3,2-*c*]thiopyran, D-80258
2,3-Dihydro-4*H*-thieno[2,3-*b*]thiopyran-4-one, D-80259
5,6-Dihydro-7*H*-thieno[3,2-*b*]thiopyran-7-one, D-80260
2,5-Dihydrothiophene, D-70270
1,2-Dihydro-2-thioxo-4*H*-3,1-benzoxazin-4-one, D-80261
7,8-Dihydro-8-thioxoguanosine, *see* M-70029
2,3-Dihydro-2-thioxopyrido[2,3-*d*]pyrimidin-4(1*H*)-one, D-60291
2,3-Dihydro-2-thioxopyrido[3,2-*d*]pyrimidin-4(1*H*)-one, D-60292
2,3-Dihydro-2-thioxopyrido[3,4-*d*]pyrimidin-4(1*H*)-one, D-60293
2,3-Dihydro-2-thioxo-4*H*-pyrido[1,2-*a*]-1,3,5-triazin-4-one, D-60294
2,3-Dihydro-2-thioxo-4(1*H*)-quinazolinone, D-60296
2,3-Dihydro-4-thioxo-2(1*H*)-quinazolinone, D-60295
Dihydrotochuinyl acetate, *in* T-70202
Dihydro-1,3,5-triazine-2,4(1*H*,3*H*)-dione, D-60297
▷ 1,2-Dihydro-3*H*-1,2,4-triazole-3-thione, D-60298
2,3-Dihydro-4-(trichloroacetyl)furan, D-70271
3,4-Dihydro-5-(trichloroacetyl)-2*H*-pyran, D-70272
Dihydrotrichostin, D-70273
2,14-Dihydrotricyclo[7.3.2.0^{5,13}]tetradeca-1,3,5,7,9,11-hexaen-2-one, *see* M-70042
2,3-Dihydro-4-(trifluoroacetyl)furan, D-70274
3,4-Dihydro-5-(trifluoroacetyl)-2*H*-pyran, D-70275
Dihydro-4-(trifluoromethyl)-2(3*H*)-furanone, D-60299
Dihydro-5-(trifluoromethyl)-2(3*H*)-furanone, D-60300
6*a*,12*a*-Dihydro-2,3,10-trihydroxy[2]benzopyrano[4,3-*b*][1]benzopyran-7(5*H*)-one, 9CI, *in* C-70200
5,6-Dihydro-6-(2,4,6-trihydroxyheneicosyl)-2*H*-pyran-2-one, D-70276
3,4-Dihydro-3,5,7-trihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-2*H*-benzopyran, *see* T-60125
6*a*,12*a*-Dihydro-3,4,10-trihydroxy-8-methoxy[2]benzopyrano[4,3-*b*][1]benzopyran-7(5*H*)-one, *in* C-70200
6*a*,12*a*-Dihydro-2,3,10-trihydroxy-8-methoxy[2]benzopyrano[4,3-*b*][1]benzopyran-7(5*H*)-one, 9CI, *in* C-70200
2,3-Dihydro-2,5,8-trihydroxy-6-methoxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, *see* F-80073
7,7*a*-Dihydro-3,6,7-trihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]oxiren-2(1*aH*)-one, D-70277
9,10-Dihydro-3,6,8-trihydroxy-1-methyl-9,10-dioxo-2-anthracenecarboxylic acid, *see* T-60332
4,10-Dihydro-3,7,8-trihydroxy-3-methyl-10-oxo-1*H*,3*H*-pyrano[4,3-*b*][1]benzopyran-9-carboxylic acid, *see* F-60081
6*a*,12*a*-Dihydro-2,3,9-trimethoxy[1]benzopyrano[3,4-*b*][1]benzopyran-12(6*H*)-one, *see* M-80196
9,10-Dihydro-3,4,6-trimethoxy-2,7-phenanthrenediol, *in* D-70246
9,10-Dihydro-5,6,7-trimethoxy-2,3-phenanthrenediol, *in* D-70246
9,10-Dihydro-5,6,8-trimethoxy-3,4-phenanthrenediol, *in* P-70034
6,7-Dihydro-6-(2,3,4-trimethoxyphenyl)-5*H*-furo[3,2-*g*][1]benzopyran-5-one, *see* N-80025
1,4-Dihydro-4,6,7-trimethyl-9*H*-imidazo[1,2-*a*]purin-9-one, D-70278
3,4-Dihydro-3,3,8*a*-trimethyl-1,6(2*H*,8*aH*)-naphthalenedione, D-60301
5,6-Dihydro-1,1,4-trimethyl-9-oxo-1*H*,4*H*-3*a*,6*a*-propanopentalene-3-carboxaldehyde, *see* P-80190
3,4-Dihydro-4,6,7-trimethyl-3-β-D-ribofuranosyl-9*H*-imidazo[1,2-*a*]purin-9-one, D-60302
3,5-Dihydro-3,5,5-trimethyl-4*H*-triazol-4-one, D-60303
3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, *see* T-80200
1,4-Dihydrotriphenylene, D-80262
4,5-Dihydro-2,4,5-triphenyl-1*H*-imidazole, D-80263
5,6-Dihydro-6-[3,5,6-tris(acetyloxy)-1-heptenyl]-2*H*-pyran-2-one, *see* H-70236
5,6-Dihydro-6-[1,2,3-tris(acetyloxy)heptyl]-2*H*-pyran-2-one, *see* B-60193
Dihydrotropidine, *in* A-70278
Dihydrotucumanoic acid, *in* T-60410
Dihydro-3-vinyl-2(3*H*)-furanone, D-70279
Dihydrovitixanthin, *in* V-80011
Dihydroxanthommatin, D-80264
7,12-Dihydroxy-8,12-abietadiene-11,14-dione, D-80265
2β,12-Dihydroxy-8,12-abietadiene-11,14-dione, *in* R-60015
3β,11-Dihydroxy-5,7,9,13-abietatetraene-2,12-dione, *see* I-80048
11,12-Dihydroxy-6,8,11,13-abietatetraen-20-oic acid, D-60305
11,12-Dihydroxy-5,8,11,13-abietatetraen-7-one, D-80266

5,12-Dihydroxy-6,8,12-abietatriene-11,14-dione, D-80267
6,12-Dihydroxy-8,11,13-abietatriene-1,7-dione, D-80268
2α,11-Dihydroxy-7,9(11),13-abietatriene-6,12-dione, *in* D-70282
11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid, D-80269
7,15-Dihydroxy-8,11,13-abietatrien-18-oic acid, D-70280
12,15-Dihydroxy-8,11,13-abietatrien-7-one, D-80270
2,11-Dihydroxy-7,9(11),13-abietatrien-12-one, D-70282
2,12-Dihydroxy-8,11,13-abietatrien-7-one, D-70281
3,12-Dihydroxy-8,11,13-abietatrien-1-one, D-60306
6,14-Dihydroxy-8,11,13-abietatrien-1-one, D-80271
3α,15-Dihydroxyalloalantolactone, *in* A-80044
2,3-Dihydroxyaniline, *see* A-70089
▷ 3,4-Dihydroxyaniline, *see* A-70090
12,13-Dihydroxy-1(10)-aromadendren-2-one, D-70283
ent-16α,17-Dihydroxy-3-atisanone, D-70284
ent-3β,16α-Dihydroxy-13-atisen-2-one, D-80272
4′,6-Dihydroxyaurone, D-80273
2,3-Dihydroxybenzaldehyde, D-70285
2,4-Dihydroxybenzeneacetaldehyde, *see* D-60369
2,5-Dihydroxybenzeneacetaldehyde, *see* D-60370
3,4-Dihydroxybenzeneacetaldehyde, *see* D-60371
4,5-Dihydroxy-1,3-benzenedicarboxylic acid, D-60307
2,5-Dihydroxybenzenemethanol, *see* D-70287
3,4-Dihydroxybenzenemethanol, *see* D-80284
β,4-Dihydroxybenzenepentanoic acid, *see* H-70142
2,2-Dihydroxy-1*H*-benz[*f*]indene-1,3(2*H*)dione, D-60308
3,4-Dihydroxybenzocyclobutene-1,2-dione, D-80274
3,5-Dihydroxybenzocyclobutene-1,2-dione, D-80275
3,6-Dihydroxybenzocyclobutene-1,2-dione, D-80276
4,5-Dihydroxybenzocyclobutene-1,2-dione, D-80277
3,6-Dihydroxybenzocyclobuten-1-one, D-80278
4,5-Dihydroxybenzocyclobuten-1-one, D-80279
4,6-Dihydroxybenzocyclobuten-1-one, D-80280
5,6-Dihydroxybenzocyclobuten-1-one, D-80281
6,7-Dihydroxy-2*H*-1-benzopyran-2-one, D-84287
(7,8-Dihydroxy-1*H*-2-benzopyran-3-yl)(2,4-dihydroxyphenyl)methanone, *in* P-70017
(6,7-Dihydroxy-1*H*-2-benzopyran-3-yl)(2,4-dihydroxyphenyl)methanone, *see* P-70017
3,6-Dihydroxy-1,2-benzoquinone, D-60309
2,4-Dihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, *in* D-10388
3-(2,4-Dihydroxybenzoyl)-7,8-dihydroxy-1*H*-2-*benzopyran*, *in* P-70017
3-(2,4-Dihydroxybenzoyl)-6,7-dihydroxy-1*H*-2-benzopyran, *see* P-70017
1-[3-(2,4-Dihydroxybenzoyl)-4,6-dihydroxy-2-(4-hydroxyphenyl)-7-benzofuranyl]-3-(4-hydroxyphenyl)-2-propen-1-one, D-70286
2,3-Dihydroxybenzyl alcohol, D-80283
2,5-Dihydroxybenzyl alcohol, D-70287
3,4-Dihydroxybenzyl alcohol, D-80284
3-(3,4-Dihydroxybenzyl)-3,7-dihydroxy-4-chromanone, *in* D-70288
3-(3,4-Dihydroxybenzyl)-3,7-dihydroxy-4-methoxychroman, *in* D-70288
3-(3,4-Dihydroxybenzyl)-7-hydroxy-4-chromanone, D-70288
2-(3,4-Dihydroxybenzylidene)-6-hydroxy-3(2*H*)-benzofuranone, *see* S-70082
3-(3,4-Dihydroxybenzylidene)-7-hydroxy-4-chromanone, *in* D-70288
3-(3,4-Dihydroxybenzyl-3,4,7-trihydroxychroman, *in* D-70288
ent-2α,3β-Dihydroxy-15-beyeren-12-one, D-80285
ent-3β,12α-Dihydroxy-15-beyeren-2-one, D-80286
ent-3β,12β-Dihydroxy-15-beyeren-2-one, *in* D-80286
7,7′-Dihydroxy-[6,8′-bi-2*H*-benzopyran]-2,2′-dione, *see* B-70093
2,3-Dihydroxybibenzyl, *see* P-60096
2,4-Dihydroxybibenzyl, *see* P-60097
2,5-Dihydroxybibenzyl, *see* P-60095
3,5-Dihydroxybibenzyl, *see* P-80100
6,7-Dihydroxy-3,7′-bicoumarin, *in* D-70006
7,7′-Dihydroxy-6,8′-bicoumarin, *see* B-70093
2,3-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione, *see* D-80274
2,4-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione, *see* D-80275
2,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione, *see* D-80276
3,4-Dihydroxybicyclo[4.2.0]octa-1,3,5-triene-7,8-dione, *see* D-80277
2,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one, *see* D-80278
3,4-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one, *see* D-80279
3,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one, *see* D-80280
4,5-Dihydroxybicyclo[4.2.0]octa-1,3,5-trien-7-one, *see* D-80281
3,4′-Dihydroxybiphenyl, *see* B-80106
1,2-Dihydroxybiphenylene, *see* B-80116
1,5-Dihydroxybiphenylene, *see* B-80117
1,8-Dihydroxybiphenylene, *see* B-80118
2,3-Dihydroxybiphenylene, *see* B-80119
2,6-Dihydroxybiphenylene, *see* B-80120
2,7-Dihydroxybiphenylene, *see* B-80121
2,2′-Dihydroxy-3,3′-bipyridine, D-80287
2,2′-Dihydroxy-4,4′-bipyridine, D-80288
2,4′-Dihydroxy-1,1′-bipyridine, D-80289
3,3′-Dihydroxy-2,2′-bipyridine, D-80290
3,3′-Dihydroxy-4,4′-bipyridine, D-80291
3,4′-Dihydroxy-2,3′-bipyridine, D-80292
4,4′-Dihydroxy-1,1′-bipyridine, D-80293
4,4′-Dihydroxy-2,2′-bipyridine, D-80294
4,4′-Dihydroxy-3,3′-bipyridine, D-80295
4,6-Dihydroxy-2,2′-bipyridine, D-80296
5,5′-Dihydroxy-2,2′-bipyridine, D-80297
5,5′-Dihydroxy-3,3′-bipyridine, D-80298
6,6′-Dihydroxy-2,2′-bipyridine, D-80299
6,6′-Dihydroxy-3,3′-bipyridine, D-80300
4,5-Dihydroxy-1,3-bis(hydroxymethyl)-2-imidazolidinone, D-80301
4,9-Dihydroxy-1,12-bis(2-hydroxypropyl)-2,6,7,11-tetramethoxy-3,10-perylenedione, *see* P-70098
1-[2,4-Dihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-3-(4-hydroxyphenyl)-2-propen-1-one, D-60310
ent-6β,17-Dihydroxy-14,15-bisnor-7,11*E*-labdadien-13-one, D-60311
6,8′-Dihydroxy-2,2′-bis(2-phenylethyl)[5,5′-bi-4*H*-1-benzopyran]-4,4′-dione, D-70289
6′,8-Dihydroxy-2,2′-bis(2-phenylethyl)-5,5′-bichromone, *see* D-70289
2,10-Dihydroxy-3-bornanone, *in* H-70173
3,10-Dihydroxyborneol, *see* H-70173
8,10-Dihydroxyborneol, *see* B-70146
▷ 3β,14β-Dihydroxy-5β-bufa-20,22-dienolide, *see* B-70289
2,3-Dihydroxybutanedioic acid, *see* T-70005
2,3-Dihydroxybutanoic acid, D-60312
3,4-Dihydroxybutanoic acid, D-60313
3,4-Dihydroxybutanoic acid γ-lactone, *see* D-60242
5-(3,4-Dihydroxy-1-butynyl)-2,2′-bithienyl, *see* B-80166
5-(3,4-Dihydroxy-1-butynyl)-5′-methyl-2,2′-bithiophene, *see* M-70054
3β,10α-Dihydroxy-4,11(13)-cadinadien-12-oic acid, *see* Z-70001
3,9-Dihydroxy-δ-cadinene, *see* C-80001
4,4′-Dihydroxychalcone, *see* B-80152
2′,β-Dihydroxychalcone, *see* H-80239
3,6-Dihydroxy-7,25-cholestadien-24-one, D-80302
▷ 3-(3,4-Dihydroxycinnamoyl)quinic acid, *see* C-70005
ent-2α,7β-Dihydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
ent-6β,15-Dihydroxy-3,13*E*-clerodadien-19-oic acid, *see* S-60003
ent-3β,4α-Dihydroxy-13-cleroden-15,16-olide, D-80303
6,7-Dihydroxycoumarin, *see* D-84287
3,4-Dihydroxycrotonolactone, *see* F-80087
3β,26-Dihydroxy-5,24*E*-cucurbitadien-11-one, *in* C-60175
3β,27-Dihydroxy-5,24*Z*-cucurbitadien-11-one, *in* C-60175
3,22-Dihydroxy-24-cycloarten-26-oic acid, D-80304
3,23-Dihydroxy-24-cycloarten-26-oic acid, D-80305
3,27-Dihydroxy-24-cycloarten-26-oic acid, D-80306
2,3-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-80307
2,4-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-80308
2,5-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-80309
2,7-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-60314
3,6-Dihydroxy-3,5-cyclohexadiene-1,2-dione, *see* D-60309
5,6-Dihydroxy-5-cyclohexene-1,2,3,4-tetrone, D-60315
ent-1α,10β-Dihydroxy-9α,15α-cyclo-20-nor-16-gibberellene-7,19-dioic acid 10,19-lactone, D-80310
3,5-Dihydroxycyclopentene, *see* C-80193
7-(4,5-Dihydroxy-2-cyclopent-1-en-3-ylaminomethyl)-7-deazaguanine, *see* Q-70004
2,3-Dihydroxy-2-cyclopropen-1-one, D-70290
4β,6α-Dihydroxy-8-daucen-10-one, *see* L-60014
1,18-Dihydroxy-14-decipien-19-oic acid, D-80311
p,p′-Dihydroxydicinammoylmethane, *in* C-80165
3,10-Dihydroxy-5,11-dielmenthadiene-4,9-dione, D-60316
2α,11α-Dihydroxy-11,13-dihydroalantolactone, *in* H-80165
8α,14-Dihydroxy-11,13-dihydromelampolide, *in* D-80320
4,6-Dihydroxy-2,5-dihydropyrimidine, *see* D-70256
4,6-Dihydroxy-3-(2,4-dihydroxybenzoyl)-7-(4-hydroxycinnamoyl)-2-(4-hydroxyphenyl)benzofuran, *see* D-70286
3′,4-Dihydroxy-3,5-dimethoxybibenzyl, *in* T-60102
2′,4′-Dihydroxy-3′,4-dimethoxychalcone, *in* H-80245
2′,6′-Dihydroxy-4,4′-dimethoxychalcone, *in* H-80246
7,7′-Dihydroxy-4,4′-dimethoxy-5,5′-dimethyl[6,8′-bi-2*H*-1-benzopyran]-2,2′-dione, *see* D-60022
5,7-Dihydroxy-3′,4′-dimethoxyflavan, *in* T-60103
4′,5-Dihydroxy-2′,7-dimethoxyflavanone, *in* T-80100
5,7-Dihydroxy-2′,8-dimethoxyflavanone, *in* T-70104

4′,5-Dihydroxy-3′,7-dimethoxyflavone, D-70291
3,4′-Dihydroxy-6,7-dimethoxyflavone, *in* T-80092
3′,7-Dihydroxy-4′,6-dimethoxyflavone, *in* T-80092
4′,7-Dihydroxy-3,6-dimethoxyflavone, *in* T-80092
3,5-Dihydroxy-2,4-dimethoxy-9*H*-fluoren-9-one, *in* T-70109
2′,4′-Dihydroxy-5,7-dimethoxyisoflavan, *in* T-80096
2′,7-Dihydroxy-3′,4′-dimethoxyisoflavan, *in* T-80095
2′,7-Dihydroxy-4′,5-dimethoxyisoflavan, *in* T-80096
2′,7-Dihydroxy-4′,6-dimethoxyisoflavan, *in* T-80098
3′,7-Dihydroxy-2′,4′-dimethoxyisoflavanone, *in* T-80099
4′,7-Dihydroxy-2′,3′-dimethoxyisoflavanone, *in* T-80099
5,7-Dihydroxy-2′,4′-dimethoxyisoflavanone, *in* T-80100
2′,7-Dihydroxy-4′,8-dimethoxyisoflavene, *in* T-80104
3′,7-Dihydroxy-2′,4′-dimethoxyisoflavene, *in* T-80103
4′,7-Dihydroxy-2′,3′-dimethoxyisoflavene, *in* T-80103
2′,5-Dihydroxy-7,8-dimethoxyisoflavone, *in* T-70110
3′,7-Dihydroxy-4′,6-dimethoxyisoflavone, *in* T-80111
4′,5-Dihydroxy-3′,7-dimethoxyisoflavone, *in* T-80109
4′,5-Dihydroxy-6,7-dimethoxyisoflavone, *in* T-80112
4′-6-Dihydroxy-5,7-dimethoxyisoflavone, *in* T-80112
4′,7-Dihydroxy-2′,5-dimethoxyisoflavone, *in* T-80106
5,7-Dihydroxy-2′,4′-dimethoxyisoflavone, *in* T-80106
5,7-Dihydroxy-2′,6-dimethoxyisoflavone, *in* T-60107
5,7-Dihydroxy-3′,4′-dimethoxyisoflavone, *in* T-80109
5,7-Dihydroxy-4′,6-dimethoxyisoflavone, *in* T-80112
5,8-Dihydroxy-2,3-dimethoxy-6,7-methylenedioxy-1,4-naphthoquinone, *in* H-60065
5,10-Dihydroxy-1,7-dimethoxy-3-methyl-1*H*-naphtho[2,3-*c*]pyran-6,9-dione, *in* T-80320
3′,5-Dihydroxy-4′,7-dimethoxyneoflavone, *in* D-80356
$\Delta^{8,8'}$-4,4′-Dihydroxy-5,5′-dimethoxy-3,3′-neolignan, *see* D-80023
2,3-Dihydroxy-5,7-dimethoxyphenanthrene, *in* T-60120
2,7-Dihydroxy-1,5-dimethoxyphenanthrene, *in* T-80114
2,7-Dihydroxy-3,4-dimethoxyphenanthrene, *in* T-80115
3,7-Dihydroxy-2,4-dimethoxyphenanthrene, *in* T-80115
5,8-Dihydroxy-6,10-dimethoxy-2-propyl-4*H*-naphtho[2,3-*b*]pyran-4-one, D-70292
5,8-Dihydroxy-6,10-dimethoxy-2-propyl-4*H*-naphtho[1,2-*b*]pyran-4-one, *in* C-70191
2,10-Dihydroxy-3,9-dimethoxypterocarpan, *in* T-80118
2,8-Dihydroxy-3,9-dimethoxypterocarpan, *in* T-80117
1,3-Dihydroxy-5,8-dimethoxyxanthone, *in* T-70123
1,8-Dihydroxy-3,5-dimethoxyxanthone, *in* T-70123
1,8-Dihydroxy-3,6-dimethoxyxanthone, *in* T-60127
2,6-Dihydroxy-3,5-dimethylbenzoic acid, D-70293
8,8′-Dihydroxy-3,3′-dimethyl[2,2′-binaphthalene]-1,1′,4,4′-tetrone, *see* B-60106
11,12-Dihydroxy-3,9-dimethyl-2,8-dioxacyclotetradeca-5,13-diene-1,7-dione, *see* C-60159
11,12-Dihydroxy-6,14-dimethyl-1,7-dioxacyclotetradeca-3,9-diene-2,8-dione, *see* C-60159
2,5-Dihydroxy-3,6-dimethyl-3,6-diphenyl-1,4-dioxan, *in* H-80240
2,5-Dihydroxy-2,5-dimethyl-1,4-dithiane, *see* D-60421
3,3′-Dihydroxy-4,5;4′,5′-dimethylenedioxybibenzyl, *in* H-60062
Dihydroxydimethylethyleneurea, *see* D-80301
5,8-Dihydroxy-2,3-dimethyl-1,4-naphthalenedione, *see* D-60317
5,8-Dihydroxy-2,3-dimethyl-1,4-naphthoquinone, D-60317
1,7-Dihydroxy-3,7-dimethyl-2,5-octadien-4-one, D-60318
2,7-Dihydroxy-1,6-dimethyl-5-vinylphenanthrene, D-70294
7β,8α-Dihydroxy-14,15-dinor-11-labden-13-one, *see* S-60052
2,3-Dihydroxy-2,3-diphenylbutanedioic acid, D-80312
3,5-Dihydroxy-1,7-diphenylheptane, *see* D-70481
1,5-Dihydroxy-1,7-diphenyl-3-heptanone, *in* D-60480
3,3-Dihydroxy-5,5-diphenyl-1,2,4,5-pentanetetrone, *in* D-60488
3,9-Dihydroxy-2,10-diprenylcoumestan, *see* E-80053
4′,7-Dihydroxy-3′,5′-di-*C*-prenylflavanone, *see* A-80009
Dihydroxydiquinone, *see* D-60315
Dihydroxy DMEU, *see* D-80301
6,12-Dihydroxy-3,7-dolabelladiene, *see* D-70541
3,11-Dihydroxy-7-drimen-6-one, D-70295
5β,20*R*-Dihydroxyecdysone, *in* H-60023
12,19-Dihydroxy-5,8,10,14-eicosatetraenoic acid, D-60319
15,20-Dihydroxy-5,8,11,13-eicosatetraenoic acid, D-70297
5,20-Dihydroxy-6,8,11,14-eicosatetraenoic acid, D-70296
5,6-Dihydroxy-7,9,11,14-eicosatetraenoic acid, D-80313
8α,15-Dihydroxy-1,3-elemadien-12,6α-olide, *see* M-80013
4,6-Dihydroxy-7,8-epoxy-20-nor-2-cembren-12-one, *in* D-70323
1,8-Dihydroxy-3,7(11)-eremophiladien-12,8-olide, D-60320
1β,10α-Dihydroxy-11β*H*-eremophilan-12,8β-olide, *in* D-80314
1,10-Dihydroxy-11(13)-eremophilen-12,8-olide, D-80314
8α,9α-Dihydroxy-10β*H*-eremophil-11-en-2-one, *in* E-70030
1,5-Dihydroxyeriocephaloide, D-60321
▷ *N,N′*-Dihydroxyethanediamide, *see* O-60048
▷ 1,3-Dihydroxy-2-(ethoxymethyl)anthraquinone, *in* D-70306
1β,8β-Dihydroxy-4,11(13)eudesmadien-12-oic acid γ-lactone, *see* I-70109
1,8-Dihydroxy-3,7(11)-eudesmadien-12,8-olide, D-60322
1,8-Dihydroxy-4(15),11(13)-eudesmadien-12,6-olide, D-80315
1,5-Dihydroxy-2,4(15),11(13)-eudesmatrien-12,8-olide, D-70298
1,6-Dihydroxy-4(15)-eudesmene, *see* E-80084
1,3-Dihydroxy-4-eudesmen-12,6-olide, D-70299
1,8-Dihydroxy-4(15)-eudesmen-12,6-olide, D-80316
2α,11α-Dihydroxy-5-eudesmen-12,8β-olide, *in* H-80165
1β,3α-Dihydroxy-4-eudesmen-12,6α-olide, *in* I-70066
1α,3α-Dihydroxy-4-eudesmen-12,6α-olide, *see* I-70066
3β,19α-Dihydroxy-24-*trans*-ferulyloxy-12-ursen-28-oic acid, *in* T-60348
2′,8-Dihydroxyflavone, D-70300
4′,7-Dihydroxyflavonol, *see* T-80300
21,27-Dihydroxy-3-friedelanone, D-70301
3α,23*R*-Dihydroxy-17,13-friedo-9β-lanosta-7,12,24*E*-trien-26-oic acid, *see* M-60010
3α,23*R*-Dihydroxy-17,14-friedo-9β-lanosta-7,14,24*E*-trien-26-oic acid, *see* M-70012
21,27-Dihydroxy-D:A-friedooleanan-3-one, *see* D-70301
2,9-Dihydroxyfuranoeremophilane, *see* F-70047
2-(8,9-Dihydroxygeranylgeranyl)-5,6-dimethyl-1,4-benzoquinone, *in* S-60010
2-(8,9-Dihydroxygeranylgeranyl)-6-methyl-1,4-benzoquinone, *in* S-60010
18,19-Dihydroxygeranylnerol, *see* B-80151
1,4-Dihydroxy-5,10(14)-germacradiene, *see* G-70009
1,3-Dihydroxy-4,10(14)-germacradien-12,6-olide, D-80317
1,3-Dihydroxy-4,9-germacradien-12,6-olide, D-80318
2,8-Dihydroxy-4,10(14)-germacradien-12,6-olide, D-80319
8,14-Dihydroxy-1(10),4-germacradien-12,6-olide, D-80320
2,8-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, D-70302
3,13-Dihydroxy-1(10),4,7(11)-germacratrien-12,6-olide, D-70303
8,9-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, D-60323
9,15-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, D-60324
▷ Dihydroxyglyoxime, *see* O-60048
2,4-Dihydroxy-5,11(13)-guaiadien-12,8-olide, D-70304
3,5-Dihydroxy-4(15),10(14)-guaiadien-12,8-olide, D-60325
4,10-Dihydroxy-2,11(13)-guaiadien-12,6-olide, D-60326
3β,9β-Dihydroxy-4(15),10(14)-guaiadien-12,6α-olide, *in* D-70305
2,8-Dihydroxy-3,10(14),11(13)-guaiatrien-12,6-olide, D-60327
3,9-Dihydroxy-10(14)-guaien-12,6-olide, D-70305
8,10-Dihydroxy-3-guaien-12,6-olide, D-60328
8,9-Dihydroxy-4,6-heptadecadiyn-3-one, D-80321
2-(3,4-Dihydroxy-1,5-heptadienyl)-6-hydroxybenzaldehyde, *see* P-60216
5,7-Dihydroxy-2′,3,4′,5′,6,8-hexamethoxyflavone, *in* O-60022
5,7-Dihydroxy-3,3′,4′,5′,6,8-hexamethoxyflavone, *in* O-70018
5,6-Dihydroxyhexanoic acid, D-60329
3,4-Dihydroxyhydratropic acid, *see* D-60372
5,7-Dihydroxy-2-[4-hydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, *see* H-70092
5,8-Dihydroxy-1-(1-hydroxyethyl)-7-methoxynaphtho[2,3-*c*]furan-4,9-dione, *see* N-60016
4,8-Dihydroxy-2-(1-hydroxyheptyl)-3,4,5,6,7,8-hexahydro-2*H*-1-benzopyran-5-one, *see* H-80057
5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6,8-dimethoxy-4*H*-1-benzopyran-4-one, *see* T-80341
▷ 1,3-Dihydroxy-2-(hydroxymethyl)-9,10-anthracenedione, *see* D-70306
▷ 1,3-Dihydroxy-2-hydroxymethylanthraquinone, D-70306
5,7-Dihydroxy-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, *see* T-80290

3β,7β-Dihydroxy-4α-hydroxymethyl-4β,14α-dimethyl-11,15-dioxo-5α-chol-8-en-24-oic acid, *see* L-60036
3β,12β-Dihydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, *in* L-60036
5,8-Dihydroxy-2-(hydroxymethyl)-6-methoxy-3-(2-oxopropyl)-1,4-naphthalenedione, *see* F-60108
5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione, *see* S-70038
5,8-Dihydroxy-2-(4-hydroxy-4-methylpentyl)naphthoquinone, *in* D-80343
3,7-Dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80300
4,5-Dihydroxy-7-(4-hydroxyphenyl)-2*H*-1-benzopyran-2-one, *see* N-80063
5,7-Dihydroxy-2-(2-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80299
▷ 5,7-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80309
7,8-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-70265
7,8-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80311
▷ 5,7-Dihydroxy-3-(4-hydroxyphenyl)-6-methoxy-4*H*-1-benzopyran-4-one, *see* T-80319
5,7-Dihydroxy-2-(4-hydroxyphenyl)-3-methoxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, *see* T-60224
5,7-Dihydroxy-3-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, *see* W-80002
1-[2,4-Dihydroxy-3-[(2-hydroxyphenyl)methyl]-6-methoxyphenyl]-3-phenyl-1-propanone, *see* U-80035
1,4-Dihydroxy-10-imino-9(10*H*)-anthracenone, *see* A-60181
5,6-Dihydroxyindole, D-70307
5,6-Dihydroxy-1*H*-indole-2-carboxylic acid, D-70308
2,3-Dihydroxy-6-iodobenzoic acid, D-60330
2,4-Dihydroxy-3-iodobenzoic acid, D-60331
2,4-Dihydroxy-5-iodobenzoic acid, D-60332
2,5-Dihydroxy-4-iodobenzoic acid, D-60333
2,6-Dihydroxy-3-iodobenzoic acid, D-60334
3,4-Dihydroxy-5-iodobenzoic acid, D-60335
3,5-Dihydroxy-2-iodobenzoic acid, D-60336
3,5-Dihydroxy-4-iodobenzoic acid, D-60337
4,5-Dihydroxy-2-iodobenzoic acid, D-60338
5,7-Dihydroxy-1(3*H*)-isobenzofuranone, D-60339
5,7-Dihydroxy-8-isobutyryl-2,2,6-trimethylchromene, *see* D-70348
4′,7-Dihydroxyisoflavanone, D-80322
4′,7-Dihydroxyisoflavone, D-80323
4,5-Dihydroxyisophthalic acid, *see* D-60307
2,5-Dihydroxy-4-isopropylbenzyl alcohol, D-70309
3α,6β-Dihydroxyivangustin, *in* I-70109
ent-7β,14α-Dihydroxy-1,16-kauradiene-3,15-dione, D-80324
ent-3α,11α-Dihydroxy-16-kaurene-6,15-dione, D-80325
ent-3β,19-Dihydroxy-15-kauren-17-oic acid, D-60341
3,15-Dihydroxy-8(17),13-labdadien-19-al, D-70310
ent-13,16-Dihydroxy-8(17),14-labdadien-18-oic acid, D-80326
2,13-Dihydroxy-8,14-labdadien-7-one, D-80327
ent-3β,15-Dihydroxy-7,13-labdadien-2-one, D-80328
8,15-Dihydroxy-13-labden-19-al, D-70311
6,15-Dihydroxy-7-labden-17-oic acid, D-60342
6,15-Dihydroxy-8-labden-17-oic acid, D-80329
7,15-Dihydroxy-8-labden-17-oic acid, D-80330
3β,15-Dihydroxy-8-labden-7-one, *in* L-70013
3,8-Dihydroxylactariusfuran, D-70312
4,8-Dihydroxylactariusfuran, D-70313
3,15-Dihydroxy-8,24-lanostadien-26-oic acid, D-80331
24,25-Dihydroxy-7,9(11)-lanostadien-3-one, D-60343
3,15-Dihydroxy-7,9(11),24-lanostatrien-26-oic acid, D-70314
7,13-Dihydroxy-2-longipinen-1-one, D-70315
7,9-Dihydroxy-2-longipinen-1-one, D-80332
3,23-Dihydroxy-20(30)-lupen-29-al, D-70316
3,23-Dihydroxy-20(29)-lupen-30-al, *see* D-70316
3,23-Dihydroxy-20(29)-lupen-28-oic acid, D-70317
1,11-Dihydroxy-20(29)-lupen-3-one, D-60345
23,30-Dihydroxy-20(29)-lupen-3-one, D-70318
6*a*,7-Dihydroxymaackiain, *in* P-80056
9,10-Dihydroxy-7-marasmen-5,13-olide, D-60346
6*a*,7-Dihydroxymedicarpin, *in* T-80120
2,4-Dihydroxy-*N*-[3-[(3-mercaptopropyl)amino]-3-oxopropyl]-3,3-dimethylbutanamide, *see* H-60090
2′,6′-Dihydroxy-4′-methoxyacetophenone, *in* T-70248
3,4-Dihydroxy-5-methoxybenzeneacetic acid, *in* T-60343
3,5-Dihydroxy-4-methoxybenzeneacetic acid, *in* T-60343
2,4-Dihydroxy-6-methoxybenzophenone, *in* T-80285
▷ 2,6-Dihydroxy-4-methoxybenzophenone, *in* T-80285
5,6-Dihydroxy-7-methoxy-2*H*-1-benzopyran-2-one, *in* T-80287
2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-10388
2,4-Dihydroxy-6-methoxy-3,5-bis(3-methyl-2-butenyl)acetophenone, *in* T-80289
2′,4-Dihydroxy-4′-methoxychalcone, *in* D-80367
2′,4′-Dihydroxy-6′-methoxychalcone, *in* P-80139
2′,6′-Dihydroxy-4′-methoxychalcone, *in* P-80139
2′,6′-Dihydroxy-4′-methoxychalcone, *in* P-80139
5,6-Dihydroxy-7-methoxycoumarin, *in* T-80287
3,7-Dihydroxy-9-methoxycoumestan, *in* T-80294
3,8-Dihydroxy-9-methoxycoumestan, *in* T-80295
7,10-Dihydroxy-12-methoxycoumestan, *in* T-80294
3,9-Dihydroxy-2-methoxycoumestone, *in* T-70249
2′,4′-Dihydroxy-6′-methoxydihydrochalcone, *in* T-80332
2,7-Dihydroxy-4-methoxy-9,10-dihydrophenanthrene, *in* P-80080
4,7-Dihydroxy-2-methoxy-9,10-dihydrophenanthrene, *in* P-80080
2′,7-Dihydroxy-4′-methoxy-4-(2′,7-dihydroxy-4′-methoxyisoflavan-5′-yl)isoflavan, D-60347
2′,4′-Dihydroxy-6′-methoxy-3′,5′-dimethyldihydrochalcone, *see* A-80156
1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone, *see* A-80156
2,4-Dihydroxy-6-methoxy-3,5-diprenylacetophenone, *in* T-80289
2,2′-Dihydroxy-3-methoxy-5,5′-di-2-propenylbiphenyl, D-80334
7,10-Dihydroxy-11-methoxydracaenone, *in* D-70546
3β,5α-Dihydroxy-6β-methoxy-7,22-ergostadiene, *in* M-70057
5,8-Dihydroxy-7-methoxyflavanone, *in* T-60321
▷ 5,7-Dihydroxy-4′-methoxyflavone, D-70319
2′,5-Dihydroxy-7-methoxyflavone, *in* T-80299
4′,7-Dihydroxy-3′-methoxyflavone, *in* T-80301
2,5-Dihydroxy-4-methoxy-9*H*-fluoren-9-one, *in* T-70261
2′,4′-Dihydroxy-7-methoxyisoflavan, *in* T-80302
4′,7-Dihydroxy-2′-methoxyisoflavan, *in* T-80302
2′,7-Dihydroxy-4′-methoxyisoflavanone, *in* T-80303
3′,7-Dihydroxy-4′-methoxyisoflavanone, *in* T-70263
5,7-Dihydroxy-4′-methoxyisoflavanone, *in* T-80304
4′,7-Dihydroxy-2′-methoxyisoflavene, *in* T-80305
4′,5-Dihydroxy-7-methoxyisoflavone, D-80335
4′,7-Dihydroxy-5-methoxyisoflavone, D-80336
5,7-Dihydroxy-4′-methoxyisoflavone, D-80337
2′,7-Dihydroxy-4′-methoxyisoflavone, *in* T-80306
3′,7-Dihydroxy-4′-methoxyisoflavone, *in* T-80308
4′,6-Dihydroxy-7-methoxyisoflavone, *in* T-80310
4′,7-Dihydroxy-2′-methoxyisoflavone, *in* T-80306
4′,7-Dihydroxy-3′-methoxyisoflavone, *in* T-80308
4′,7-Dihydroxy-6-methoxyisoflavone, *in* T-80310
7,8-Dihydroxy-4′-methoxyisoflavone, *in* T-70265
7,8-Dihydroxy-4′-methoxyisoflavone, *in* T-80311
1,8-Dihydroxy-6-methoxy-2-methylanthraquinone, *in* T-70269
3,8-Dihydroxy-6-methoxy-1-methylanthraquinone-2-carboxylic acid, *in* T-80323
1,8-Dihydroxy-3-methoxy-7-methylanthraquinone(incorr.), *in* T-70269
1-[2,6-Dihydroxy-4-methoxy-3-(3-methyl-2-butenyl)phenyl]-3-phenyl-2-propen-1-one, *see* I-80100
1,6-Dihydroxy-3-methoxy-2-(3-methyl-2-butenyl)xanthone, *in* T-80325
5,7-Dihydroxy-6-methoxy-3′,4′-methylenedioxyisoflavone, *in* P-80043
3,6*a*-Dihydroxy-4-methoxy-8,9-methylenedioxypterocarpan, *in* P-80053
1,3-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan, *in* P-80051
2,5-Dihydroxy-8-methoxy-3-methyl-6,7-methylenedioxy-1,4-naphthoquinone, *in* T-60333
2′,6′-Dihydroxy-4′-methoxy-3′-(3-methyl-6-methylethyl-2-cyclohexenyl)chalcone, *see* D-80338
1-[2,6-Dihydroxy-4-methoxy-3-[3-methyl-6-(1-methylethyl)-2-cyclohexen-1-yl]phenyl]-3-phenyl-2-propen-1-one, *see* D-80338
1-[3-[[2,6-Dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxy-5-methylphenyl]-1-butanone, *see* A-80039
2,5-Dihydroxy-4-methoxyphenanthrene, *in* P-60071
2,6-Dihydroxy-7-methoxy-5*H*-phenanthro[4,5-*bcd*]pyran-5-one, *see* F-80009
3,4-Dihydroxy-5-methoxyphenylacetic acid, *in* T-60343
3,5-Dihydroxy-4-methoxyphenylacetic acid, *in* T-60343
▷ 5,7-Dihydroxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, *see* D-70319
5,7-Dihydroxy-3-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, *see* D-80337
2′,7-Dihydroxy-4′-methoxy-3-phenylcoumarin, *in* D-80364
1-(2,4-Dihydroxy-3-methoxyphenyl)-3-(3,4-dihydroxyphenyl)-2-propen-1-one, *in* D-80372
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone, *in* H-80244

3-(2,4-Dihydroxy-6-methoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* H-80243
1-(2,4-Dihydroxy-3-methoxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one, *in* H-80245
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one, *in* H-80246
2-(2,4-Dihydroxy-3-methoxyphenyl)-5,6-methylenedioxybenzofuran, *in* D-80389
1-(2,4-Dihydroxy-6-methoxyphenyl)-3-phenyl-1-propanone, *in* T-80332
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-1-propanone, *in* T-80332
1-(2,4-Dihydroxy-6-methoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
2′,6′-Dihydroxy-4′-methoxy-β-phenylpropiophenone, *in* T-80332
1-(2,3-Dihydroxy-4-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)ethane, *in* T-60344
1-(2,3-Dihydroxy-4-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)ethylene, *in* T-60344
2′,6′-Dihydroxy-4′-methoxy-3′-(1-p-menthen-3-yl)chalcone, D-80338
3β,12-Dihydroxy-13-methoxy-8,11,13-podocarpatrien-7-one, *see* N-80028
2′,6′-Dihydroxy-4′-methoxy-3′-prenylchalcone, *see* I-80100
4′,7-Dihydroxy-5-methoxy-8-*C*-prenylflavanone, *see* I-80099
3,6*a*-Dihydroxy-9-methoxy-10-prenylpterocarpan, *see* C-80156
3,9-Dihydroxy-1-methoxy-10-prenylpterocarpan, *in* P-80076
5,8-Dihydroxy-10-methoxy-2-propyl-4*H*-naphtho[1,2-*b*]pyran-4-one, *see* C-70191
5,10-Dihydroxy-8-methoxy-2-propyl-4*H*-*naphtho*[1,2-*b*]pyran-4-one, 9CI, *in* C-70191
3,6*a*-Dihydroxy-9-methoxypterocarpan, *in* T-80337
6*a*,9-Dihydroxy-3-methoxypterocarpan, *in* T-80337
3,10-Dihydroxy-9-methoxypterocarpan, *in* T-80338
3,4-Dihydroxy-9-methoxypterocarpan, *in* T-80336
3,9-Dihydroxy-10-methoxypterocarpan, *in* T-80338
9,10-Dihydroxy-5-methoxy-2*H*-pyrano[2,3,4-*kl*]xanthen-9-one, *in* T-70273
α,4-Dihydroxy-3-methoxytoluene, *in* D-80284
5,7-Dihydroxy-6-methoxy-3-(2,4,5-trimethoxyphenyl)-4*H*-1-benzopyran-4-one, *in* H-80069
▷ 1,3-Dihydroxy-7-methoxyxanthone, *in* T-80347
1,5-Dihydroxy-6-methoxyxanthone, *in* T-60349
1,6-Dihydroxy-5-methoxyxanthone, *in* T-60349
▷ 1,7-Dihydroxy-3-methoxyxanthone, *in* T-80347
3,7-Dihydroxy-1-methoxyxanthone, *in* T-80347
5,6-Dihydroxy-1-methoxyxanthone, *in* T-60349
3,4-Dihydroxy-α-methylbenzeneacetic acid, *see* D-60372
8,9-Dihydroxy-1-methyl-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, *see* M-70161
4,5-Dihydroxy-2-methylbenzoic acid, D-80339
8,11-Dihydroxy-12*b*-methyl-1*H*-benzo[6,7]phenanthro[10,1-*bc*]furan-3,6(2*H*,12*bH*)-dione, *see* H-60002
4,7-Dihydroxy-5-methyl-2*H*-1-benzopyran-2-one, D-60348
▷ 2,3-Dihydroxy-5-methyl-1,4-benzoquinone, D-70320
5,7-Dihydroxy-7-(3-methyl-2-butenyl)-8-(2-methyl-2-oxopropyl)-3-propyl-2*H*-1-benzopyran-2-one, D-80340
3,6-Dihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]-2,7(1*aH*,7*aH*)-dione, *in* D-70277
2-[3,4-Dihydroxy-5-(3-methyl-2-butenyl)phenyl]-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* S-70041
[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-5,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* L-80028
9-(2,3-Dihydroxy-2-methylbutoxy)-4-methoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, *see* B-80296
N-(2,3-Dihydroxy-3-methylbutyl)acetamide, *in* A-60216
7-(2′,3′-Dihydroxy-3′-methylbutyloxy)-6-methoxy-2*H*-1-benzopyran-2-one, *in* H-80189
5,7-Dihydroxy-8-(2-methylbutyryl)-4-pentylcoumarin, *see* D-80342
4,7-Dihydroxy-5-methylcoumarin, *see* D-60348
2,3-Dihydroxy-5-methyl-2,5-cyclohexadiene-1,4-dione, *see* D-70320
1,3-Dihydroxy-4-methyl-6,8-decadien-5-one, D-70321
3,5-Dihydroxy-6,7-methylenedioxyflavanone, *in* T-60105
2′,7-Dihydroxy-4′,5′-methylenedioxyisoflavan, *in* T-80097
2′,7-Dihydroxy-4′,5′-methylenedioxyisoflavanone, *in* T-80101
4′,5-Dihydroxy-6,7-methylenedioxyisoflavone, D-80341
2′,5-Dihydroxy-6,7-methylenedioxyisoflavone, *in* T-60107
2′,7-Dihydroxy-3′,4′-methylenedioxyisoflavone, *in* T-80105
5,7-Dihydroxy-3′,4′-methylenedioxyisoflavone, *in* T-80109
2′,7-Dihydroxy-4′,5′-methylenedioxy-3-phenylcoumarin, *in* H-80261
3,6*a*-Dihydroxy-8,9-methylenedioxypterocarpan, *in* T-80121
3,4-Dihydroxy-8,9-methylenedioxypterocarpan, *in* T-80119
2-(1,2-Dihydroxy-1-methylethyl)-2,3-dihydro-5-benzofurancarboxaldehyde, *in* D-70214
2,4-Dihydroxy-3-methyl-2-hexenoic acid γ-lactone, *see* E-60051
4,4′-Dihydroxy-α-methylhydrobenzoin, *see* B-70147
5,7-Dihydroxy-6-methyl-1(3*H*)-isobenzofuranone, D-60349
4,7-Dihydroxy-9-methyl-10*H*-isobenzofuro[5,6-*b*][1,4]benzodioxepin-3,10(1*H*)-dione, *see* V-80004
1,2-Dihydroxy-3-methylnaphthalene, *see* M-60093
1,2-Dihydroxy-6-methylnaphthalene, *see* M-60095
1,3-Dihydroxy-2-methylnaphthalene, *see* M-60091
1,5-Dihydroxy-2-methylnaphthalene, *see* M-60092
2,4-Dihydroxy-1-methylnaphthalene, *see* M-60094
3,5-Dihydroxy-2-methyl-1,4-naphthalenedione, *see* D-60350
5,6-Dihydroxy-2-methyl-1,4-naphthalenedione, *see* D-60351
3,5-Dihydroxy-2-methyl-1,4-naphthoquinone, D-60350
5,6-Dihydroxy-2-methyl-1,4-naphthoquinone, D-60351
4,5-Dihydroxy-3-methyl-7-oxabicyclo[4.1.0]hept-3-en-2-one, *see* T-70009
5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-4-one, D-80342
5,7-Dihydroxy-8-(2-methyl-1-oxopropyl)-7-prenyl-3-propylcoumarin, *see* D-80340
1-[4,5-Dihydroxy-*N*-(12-methyl-1-oxotetradecyl)ornithine]-5-serineechinocandin B, *see* M-70157
2,5-Dihydroxy-3-methylpentanoic acid, D-60353
2-(1,4-Dihydroxy-4-methylpentyl)-5,8-dihydroxy-1,4-naphthoquinone, D-80343
16-(2,5-Dihydroxy-3-methylphenyl)-2,6,10,19-tetramethyl-2,6,10,14-hexadecatetraene-4,12-dione, *in* H-70225
5,7-Dihydroxy-6-methylphthalide, *see* D-60349
3,4-Dihydroxy-2-methylpyridine, *see* H-80214
8′,9′-Dihydroxy-5-methylsargaquinone, *in* S-60010
2,4-Dihydroxy-1-naphthalenamine, *see* A-80118
2,5-Dihydroxy-1,4-naphthalenedione, *see* D-60354
2,8-Dihydroxy-1,4-naphthalenedione, *see* D-60355
▷ 5,8-Dihydroxy-1,4-naphthalenedione, *see* D-60356
8,9-Dihydroxynaphtho[2,3-*c*]furan-1(3*H*)-one, *see* S-80039
2,5-Dihydroxy-1,4-naphthoquinone, D-60354
2,8-Dihydroxy-1,4-naphthoquinone, D-60355
▷ 5,8-Dihydroxy-1,4-naphthoquinone, D-60356
3,5-Dihydroxy-1,4-naphthoquinone, *see* D-60355
1,4-Dihydroxy-2-naphthylamine, *see* A-80114
1,6-Dihydroxy-2-naphthylamine, *see* A-80115
2,4-Dihydroxy-1-naphthylamine, *see* A-80118
2,6-Dihydroxy-1-naphthylamine, *see* A-80112
2,7-Dihydroxy-1-naphthylamine, *see* A-80113
3,4-Dihydroxy-1-naphthylamine, *see* A-80117
3,4-Dihydroxy-2-naphthylamine, *see* A-80116
4,6-Dihydroxy-1-naphthylamine, *see* A-80120
4,8-Dihydroxy-1-naphthylamine, *see* A-80119
5,6-Dihydroxy-1-naphthylamine, *see* A-80121
5,6-Dihydroxy-2-naphthylamine, *see* A-80124
6,7-Dihydroxy-2-naphthylamine, *see* A-80123
18,19-Dihydroxynerylgeraniol, *see* H-70179
2′,3′-Dihydroxy-6′-nitroacetophenone, D-60357
2′,5′-Dihydroxy-4′-nitroacetophenone, D-70322
3′,6′-Dihydroxy-2′-nitroacetophenone, D-60358
4′,5′-Dihydroxy-2′-nitroacetophenone, D-60359
4,5-Dihydroxy-2-nitrobenzoic acid, D-60360
1,2-Dihydroxy-4-nitronaphthalene, *see* N-80053
1,4-Dihydroxy-2-nitronaphthalene, *see* N-80050
1,5-Dihydroxy-2-nitronaphthalene, *see* N-80051
1,5-Dihydroxy-4-nitronaphthalene, *see* N-80054
1,7-Dihydroxy-2-nitronaphthalene, *see* N-80052
2,3-Dihydroxy-6-nitronaphthalene, *see* N-80056
2,6-Dihydroxy-1-nitronaphthalene, *see* N-80048
4,6-Dihydroxy-1-nitronaphthalene, *see* N-80055
1-(2,3-Dihydroxy-6-nitrophenyl)ethanone, *see* D-60357
1-(2,5-Dihydroxy-4-nitrophenyl)ethanone, *see* D-70322
1-(3,6-Dihydroxy-2-nitrophenyl)ethanone, *see* D-60358
1-(4,5-Dihydroxy-2-nitrophenyl)ethanone, *see* D-60359
12,16-Dihydroxy-20-nor-5(10),6,8,12-abietatetraene-11,14-dione, *see* N-60017
4,6-Dihydroxy-20-nor-2,7-cembradien-12-one, D-70323

ent-10β,13-Dihydroxy-20-nor-16-gibberellene-7,19-dioic acid 19,10-lactone, *see* G-70011
5,7-Dihydroxy-13-nor-8-marasmanone, D-60361
5,8-Dihydroxy-13-nor-7-marasmanone, D-60362
3,23-Dihydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, D-70324
3,24-Dihydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, D-80344
3,18-Dihydroxy-28-nor-12-oleanen-16-one, D-60363
ent-15,16-Dihydroxy-19-nor-4-rosen-3-one, *see* N-60061
3β,5α-Dihydroxy-24-nor-4(23),18-ursadien-28-oic acid, *see* K-80001
4,14-Dihydroxyoctadecanoic acid, D-80345
2,3-Dihydroxy-12-oleanene-23,28-dioic acid, D-80346
1,3-Dihydroxy-12-oleanen-29-oic acid, D-70325
3,19-Dihydroxy-12-oleanen-28-oic acid, D-70327
3,29-Dihydroxy-12-oleanen-28-oic acid, D-80347
3,6-Dihydroxy-12-oleanen-29-oic acid, D-70326
1,11-Dihydroxy-18-oleanen-3-one, D-60364
2,10-Dihydroxyondetianone, *see* D-80391
8β,9α-Dihydroxy-4,10(14)-oplopadien-3-one, *in* O-70042
10,15-Dihydroxy-4-oplopanone, D-80348
3,5-Dihydroxy-1,2,4-oxadiazole, *see* O-70060
▷ *N,N'*-Dihydroxyoxamide, *see* O-60048
6,17-Dihydroxy-15,17-oxido-16-spongianone, D-60365
11,12-Dihydroxy-7-oxo-8,11,13-abietatrien-20-oic acid, *in* T-60337
ent-13*R*-14*R*-Dihydroxy-3-oxo-15-atisen-17-al, D-80349
6,7-Dihydroxy-3-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-2*H*-1-benzopyran-2-one, *in* D-70006
6-[4-(5,7-Dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl)phenoxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* H-60082
3,5-Dihydroxy-19-oxo-14,20(22)-cardadienolide, D-80350
4,5-Dihydroxy-3-oxo-1-cyclohexenecarboxylic acid, D-70328
2,3-Dihydroxy-6-oxo-23,24-dinor-1,3,5(10),7-friedelatetraen-29-oic acid, D-80351
1,5-Dihydroxy-2-oxo-3,11(13)-eudesmadien-12,8-olide, D-70329
2,3-Dihydroxy-6-oxo-D:A-friedo-24-noroleana-1,3,5(10),7-tetraen-23,29-dioic acid, *see* D-70027
2,9-Dihydroxy-8-oxo-1(10),4,11(13)-germacratrien-12,6-olide, D-60366
3,15-Dihydroxy-23-oxo-7,9(11),24-lanostatrien-26-oic acid, D-70330
19,29-Dihydroxy-3-oxo-12-oleanen-28-oic acid, D-70331
11,15-Dihydroxy-9-oxo-5,13-prostadienoic acid, D-60367
3,5-Dihydroxy-4-oxo-4*H*-pyran-2-carboxylic acid, D-60368
3,6-Dihydroxy-2-(1-oxo-10-tetradecenyl)-2-cyclohexen-1-one, D-70332
2,19-Dihydroxy-3-oxo-1,12-ursadien-28-oic acid, D-80352
22,23-Dihydroxy-3-oxo-12-ursen-30-oic acid, D-70333
5α,20-Dihydroxy-1-oxo-20R,22R-witha-2,6,24-trienolide, *see* W-80003
3,5-Dihydroxy-3',4',5',7,8-pentamethoxyflavone, *in* H-70021
3',5-Dihydroxy-4',5',6,7,8-pentamethoxyflavone, *in* H-80029
5,7-Dihydroxy-3,3',4',5',8-pentamethoxyflavone, *in* H-70021
5,7-Dihydroxy-3',4',5',6,8-pentamethoxyflavone, *in* H-80029
3,4-Dihydroxypentanoic acid, D-80353
6,7-Dihydroxy-1,12-perylenedione, D-80354
6,12-Dihydroxy-1,7-perylenedione, *in* D-80354
4,5-Dihydroxyphenanthrene, *see* P-70048
2,4-Dihydroxyphenylacetaldehyde, D-60369
2,5-Dihydroxyphenylacetaldehyde, D-60370
3,4-Dihydroxyphenylacetaldehyde, D-60371
2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-5,7-diol, *see* T-60103
2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-3,5,7-triol, *see* P-70026
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran, *see* T-70105
3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, *see* K-80010
3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5-hydroxy-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b'*]dipyran-4-one, *see* D-80021
3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5-hydroxy-7-methoxy-6-methyl-4*H*-1-benzopyran-4-one, *see* O-80050
2-(2,4-Dihydroxyphenyl)-5,6-dihydroxybenzofuran, D-80355
4-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2*H*-1-benzopyran-2-one, D-70334
4-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2*H*-1-benzopyran-2-one, D-80356
2-(2,3-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* T-60106
2-(2,6-Dihydroxyphenyl)-5,6-dihydroxy-4*H*-1-benzopyran-4-one, *see* T-70107
2-(2,6-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* T-50153
3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* T-80106
3-(3,4-Dihydroxyphenyl)-5,7,8-dihydroxy-4*H*-1-benzopyran-4-one, *see* P-80045
3-(3,4-Dihydroxyphenyl)-6,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* T-80111
4-(3,4-Dihydroxyphenyl)-5,7-dihydroxycoumarin, *see* D-70334
4-(3,4-Dihydroxyphenyl)-5,7-dihydroxycoumarin, *see* D-80356
1-(2,4-Dihydroxyphenyl)-3-[3,4-dihydroxy-2-(3,7-dimethyl-2,6-octadienyl)phenyl]-1-propanone, D-80357
2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, *see* T-80116
4-(3,4-Dihydroxyphenyl)-6,7-dihydroxy-2-naphthalenecarboxylic acid, D-80358
1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethane, D-80359
1-(2,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene, D-70335
1-(3,4-Dihydroxyphenyl)-2-(3,4,5-dihydroxyphenyl)ethylene, D-80360
1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene, D-80361
1-(2,6-Dihydroxyphenyl)-9-(3,4-dihydroxyphenyl)-1-nonanone, *in* M-70007
1-(2,4-Dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)propane, D-70336
1-(2,4-Dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)-2-propen-1-one, D-80362
2-(2,4-Dihydroxyphenyl)-5,6-dimethoxybenzofuran, *in* D-80355
2-(3,5-Dihydroxyphenyl)-5,6-dimethoxybenzofuran, *in* M-60146
3-(2,4-Dihydroxyphenyl)-5,7-dimethoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, *see* G-80031
1-(3,4-Dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)ethane, *in* D-80359
3-(2,4-Dihydroxyphenyl)-5,7-dimethoxy-6-prenylcoumarin, *see* G-80031
4-[2-(3,5-Dihydroxyphenyl)ethenyl]-1,2-benzenediol, *see* D-80361
4-[2-(3,5-Dihydroxyphenyl)ethenyl]-1,3-benzenediol, *see* D-70335
4-[2-(3,5-Dihydroxyphenyl)ethyl]-1,2-benzenediol, *see* D-80359
5-[2-(3,4-Dihydroxyphenyl)ethyl]-1,2,3-benzenetriol, *see* D-80371
5-[2-(3,4-Dihydroxyphenyl)ethyl]-1,2,3-benzenetriol, *see* P-60044
6-(2,3-Dihydroxyphenylethyl)-2-[(4-hydroxymethyl)-3-pentenyl]-2-methylchromene, *see* T-70008
2-(3,4-Dihydroxyphenyl)-6-β-D-glucopyranosyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one, *see* I-80068
2,4-Dihydroxyphenyl 1-hydro-7,8-dihydroxy-2-oxa-3-naphthyl ketone, *in* P-70017
2-(2,4-Dihydroxyphenyl)-6-hydroxybenzofuran, D-80363
2-(3,5-Dihydroxyphenyl)-6-hydroxybenzofuran, *see* M-60146
3-(2,4-Dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran-2-one, D-80364
3-(2,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, *see* T-70264
3-(2,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, *see* T-80306
3-(3,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, *see* T-80308
3-(2,4-Dihydroxyphenyl)-7-hydroxycoumarin, *see* D-80364
4-(3,4-Dihydroxyphenyl)-8-hydroxy-5,7-dimethoxycoumarin, *in* D-80370
3-(2,4-Dihydroxyphenyl)-5-hydroxy-8,8-dimethyl-4*H*, 8*H*-benzo[1,2-*b*:3,4-*b'*]dipyran-4-one, *see* P-80014
7-(2,4-Dihydroxyphenyl)-5-hydroxy-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b'*]dipyran-6-one, *see* P-80015
2-(3,5-Dihydroxyphenyl)-5-hydroxy-6-methoxybenzofuran, *in* M-60146
4-(3,4-Dihydroxyphenyl)-7-hydroxy-5-methoxycoumarin, *in* D-80356
1-(3,5-Dihydroxyphenyl)-2-(3-hydroxy-4-methoxyphenyl)ethylene, *in* D-80361
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)-2-propen-1-one, *in* D-80362
3-[4-(3,4-Dihydroxyphenyl)-3-hydroxy-5-oxo-2-(5*H*)furanylidene]-5,6-dihydroxy-2(3*H*)-benzofuranone, *see* V-80003
1-(3,4-Dihydroxyphenyl)-2-(3-hydroxyphenyl)ethane, *see* T-60316
1-(2,6-Dihydroxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone, *in* M-70007
1-(3,4-Dihydroxyphenyl)-5-(4-hydroxyphenyl)-1-penten-4-yne, D-80365
3-(2,4-Dihydroxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, D-80366
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one, D-80367
3,5-Dihydroxy-4-phenylisoxazole, D-70337
1-(2,4-Dihydroxyphenyl)-2-(4-methoxyphenyl)-1-propanone, *see* A-80155
2-(2,4-Dihydroxyphenyl)-7-methoxy-5-(1-propenyl)benzofuran, *in* H-60214
3-[(3,4-Dihydroxyphenyl)methyl]-2,3-dihydro-7-hydroxy-4*H*-1-benzopyran-4-one, *see* D-70288
2-[(3,4-Dihydroxyphenyl)methylene]-4,6-dihydroxy-3(2*H*)-benzofuranone, *see* A-80188
2-(2,4-Dihydroxyphenyl)-5,6-methylenedioxybenzofuran, *in* D-80355
9-(3,4-Dihydroxyphenyl)-1-(3,4-methylenedioxyphenyl)-1-nonanone, *in* M-70007
2-[(3,4-Dihydroxyphenyl)methylene]-6-hydroxy-3(2*H*)-benzofuranone, *see* S-70082
1-(2,6-Dihydroxyphenyl)-4-methyl-4-tridecen-1-one, D-80368
1-(3,4-Dihydroxyphenyl)-2-nitroethylene, *see* N-70049
2-(3,4-Dihydroxyphenyl)-3,5,6,7,8-pentahydroxy-4*H*-1-benzopyran-4-one, *see* H-80028
1-(3,5-Dihydroxyphenyl)-2-phenylethane, *see* P-80100

1-(2,5-Dihydroxyphenyl)-2-phenylethylene, *see* D-80380
1-(3,4-Dihydroxyphenyl)-2-phenylethylene, *see* D-80382
1-(3,5-Dihydroxyphenyl)-2-phenylethylene, *see* D-80384
1-(2,6-Dihydroxyphenyl)-9-phenyl-1-nonanone, *see* M-70007
2-(3,4-Dihydroxyphenyl)propanoic acid, D-60372
2-(2,4-Dihydroxyphenyl)-5-(1-propenyl)benzofuran, *in* H-60214
2-(3,4-Dihydroxyphenyl)propionic acid, *see* D-60372
4-[3-[(2,4-Dihydroxyphenyl)propyl]]-1,2-benzenediol, *see* D-70336
3,5-Dihydroxy-4-phenylpyrazole, D-80369
1-(2,6-Dihydroxyphenyl)-1-tetradecanone, D-70338
1-(3,4-Dihydroxyphenyl)-1,2,3,4-tetrahydro-7-hydroxy-6-methoxy-2,3-naphthalenedimethanol, *see* I-60139
3-(3,4-Dihydroxyphenyl)-5,6,7-trihydroxy-4*H*-1-benzopyran-4-one, *see* P-80043
3-(3,4-Dihydroxyphenyl)-6,7,8-trihydroxy-4*H*-1-benzopyran-4-one, *see* P-80046
4-(3,4-Dihydroxyphenyl)-5,7,8-trihydroxycoumarin, D-80370
1-(3,4-Dihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethane, D-80371
1-(3,4-Dihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethane, *see* P-60044
3-(3,4-Dihydroxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, D-80372
3-(3,4-Dihydroxyphenyl)-1-(2,4,5-trihydroxyphenyl)-2-propen-1-one, D-70339
1-(3,4-Dihydroxyphenyl)-2-(3,4,5-trimethoxyphenyl)ethane, *in* D-80371
3,4-Dihydroxyphthalaldehydic acid, *see* F-60070
5,6-Dihydroxyphthalaldehydic acid, *see* F-60073
5,7-Dihydroxyphthalide, *see* D-60339
ent-3β,12β-Dihydroxy-8(14),15-pimaradien-2-one, *in* P-80146
ent-3β,14α-Dihydroxy-7,9(11),15-pimaratriene-2,12-dione, D-80373
1α,5α-Dihydroxypinnatifidin, *in* D-70329
12,13-Dihydroxy-8,11,13-podocarpatriene-3,7-dione, D-80374
3,9-Dihydroxy-2-prenylcoumestan, *see* P-80186
4′,7-Dihydroxy-3′-*C*-prenylflavanone, *see* A-80007
5,7-Dihydroxy-8-prenylflavanone, *see* G-70015
2-(3,5-Dihydroxy-4-prenylphenyl)-6-hydroxybenzofuran, *in* M-60146
3,9-Dihydroxy-10-prenylpterocarpan, *see* P-80076
3,4-Dihydroxyproline, *see* D-70342
5-(1,3-Dihydroxypropyl)-2-isopropenyl-2,3-dihydrobenzofuran, D-70340
3,9-Dihydroxypterocarpan, D-60373
3,9-Dihydroxypterocarpene, D-80376
2,3-Dihydroxypyridine, *in* H-60223
2,4-Dihydroxypyridine, *in* H-60224
2,5-Dihydroxypyridine, *in* H-60225
2,6-Dihydroxypyridine, *in* H-60226
3,4-Dihydroxypyridine, *in* H-60227
4,6-Dihydroxy-2(1*H*)-pyridinone, D-70341
2,4-Dihydroxypyrido[2,3-*d*]pyrimidine, *see* P-60236
2,4-Dihydroxypyrimido[4,5-*b*]quinoline, *see* P-60245
3,4-Dihydroxy-2-pyrrolidinecarboxylic acid, D-70342
3,4-Dihydroxy-2,5-pyrrolidinedione, D-80377
5,8-Dihydroxyquinazoline, *see* Q-60002
2,3-Dihydroxyquinoxaline, *see* D-60279
5,8-Dihydroxyquinoxaline, *see* Q-60008
6,7-Dihydroxyquinoxaline, *see* Q-60009
8′,9′-Dihydroxysargaquinone, *in* S-60010
20,24-Dihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, D-70343
20,25-Dihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, D-70344
16α,19α-Dihydroxy-2,3-seco-12-ursene-2,3,28-trioic acid, *see* M-80199
3,19-Dihydroxy-13(16),14-spongiadien-2-one, D-70345
2α,19-Dihydroxy-13(16),14-spongiadien-3-one, *see* I-60137
2α,19-Dihydroxy-13(16),14-spongiadien-3-one, *in* H-70220
7,12-Dihydroxysterpurene, D-70346
9,12-Dihydroxysterpurene, D-70347
2,2′-Dihydroxystilbene, D-80378
2,4′-Dihydroxystilbene, D-80379
2,5-Dihydroxystilbene, D-80380
3,3′-Dihydroxystilbene, D-80381
3,4-Dihydroxystilbene, D-80382
3,4′-Dihydroxystilbene, D-80383
3,5-Dihydroxystilbene, D-80384
4,4′-Dihydroxystilbene, D-80385
2,4-Dihydroxystyrene, *see* V-70010
Di-(*p*-hydroxystyryl)methane, *see* B-60162
2,3-Dihydroxysuccinimide, *see* D-80377
2α,3β-Dihydroxy-28,20β-taraxastanolide, *see* C-80026
2α,7-Dihydroxytaxodone, *in* D-70282
3,9-Dihydroxytetradecanoic acid, D-80386
2,3-Dihydroxy-3,4,4′,5-tetramethoxybibenzyl, *in* T-60344
3′,5-Dihydroxy-4′,6,7,8-tetramethoxyflavone, D-60375
5,7-Dihydroxy-3′,4′,6,8-tetramethoxyflavone, D-60376
4′,5-Dihydroxy-3,3′,6,7-tetramethoxyflavone, *in* H-80067
4′,5-Dihydroxy-3,3′,6,7-tetramethoxyflavone, *in* H-80067
4′,5-Dihydroxy-3′,5′,6,7-tetramethoxyflavone, *in* H-70081
5′,5′-Dihydroxy-2′,3,7,8-tetramethoxyflavone, *in* H-70080
5,7-Dihydroxy-3′,4′,5′,6-tetramethoxyflavone, *in* H-70081
2′,6-Dihydroxy-3′,4′,7,8-tetramethoxyisoflavan, *in* H-80068
5,7-Dihydroxy-2′,4′,5′,6-tetramethoxyisoflavone, *in* H-80069
5,7-Dihydroxy-2′,4′,5′,8-tetramethoxyisoflavone, *in* H-80070
5,7-Dihydroxy-3′,4′,5′,6-tetramethoxyisoflavone, *in* H-80071
3,7-Dihydroxy-1,2,5,6-tetramethoxyphenanthrene, *in* H-60066
2,8-Dihydroxy-3,4,9,10-tetramethoxypterocarpan, *in* H-80072
2-(5,16-Dihydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-6-methyl-1,4-benzenediol, *in* H-70225
5,8-Dihydroxy-2,3,6,7-tetramethyl-1,4-naphthalenedione, *see* D-60377
5,8-Dihydroxy-2,3,6,7-tetramethyl-1,4-naphthoquinone, D-60377
3,8-Dihydroxy-13,14,15,16-tetranor-12-labdanoic acid, D-80387
7,12-Dihydroxy-3,11,15,23-tetraoxo-8,20(22)-lanostadien-26-oic acid, D-60378
7,20-Dihydroxy-3,11,15,23-tetraoxo-8-lanosten-26-oic acid, D-60379
3,6-Dihydroxy-1,2,4,5-tetrazine, *see* D-70268
α,4-Dihydroxytoluene, *see* H-80114
5,6-Dihydroxy-*p*-toluquinone, *see* D-70320
3,4-Dihydroxy-2,5-toluquinone, *see* D-70320
ent-3β,18-Dihydroxy-19-trachylobanoic acid, D-80388
5,6-Dihydroxy-2-(2,3,4-trihydroxyphenyl)benzofuran, D-80389
5,7-Dihydroxy-3-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* P-80041
6,7-Dihydroxy-3-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* P-80042
6,7-Dihydroxy-3-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* P-80044
5,8-Dihydroxy-2,3,6-trimethoxy-1,4-benzoquinone, *in* P-70033
3,5-Dihydroxy-3′,4,4′-trimethoxybibenzyl, *in* D-80360
4,4′-Dihydroxy-3,3′,5-trimethoxybibenzyl, *in* D-80360
4,4′-Dihydroxy-3,3′,5-trimethoxybibenzyl, *in* P-60044
2′,5′-Dihydroxy-3′,4′,6′-trimethoxychalcone, *in* P-80050
3,3′-Dihydroxy-4′,5,7-trimethoxyflavan, *in* P-70026
3,4′-Dihydroxy-3′,5,7-trimethoxyflavan, *in* P-70026
3′,5-Dihydroxy-4′,6,7-trimethoxyflavanone, *in* P-70028
3,4′-Dihydroxy-5,6,7-trimethoxyflavone, *in* P-80035
3,5-Dihydroxy-4′,6,7-trimethoxyflavone, *in* P-80035
4′,5-Dihydroxy-3,6,7-trimethoxyflavone, *in* P-80035
4′,5-Dihydroxy-3,6,8-trimethoxyflavone, *in* P-60048
5′,6-Dihydroxy-2′,3,5,7-trimethoxyflavone, *in* H-60064
5,6-Dihydroxy-3,4′,8-trimethoxyflavone, *in* P-60048
5,7-Dihydroxy-3,4′-6-trimethoxyflavone, *in* P-80035
5,7-Dihydroxy-3,6,8-trimethoxyflavone, *in* P-70031
3′,7-Dihydroxy-2′,4′,8-trimethoxyisoflavan, *in* P-80038
3′,8-Dihydroxy-4′,7,8-trimethoxyisoflavone, *in* P-80046
4′,5-Dihydroxy-2′,5′,7-trimethoxyisoflavone, *in* P-80041
5,7-Dihydroxy-3′,4′,7-trimethoxyisoflavone, *in* P-80043
5,7-Dihydroxy-3′,4′,8-trimethoxyisoflavone, *in* P-80045
2,6-Dihydroxy-1,5,7-trimethoxyphenanthrene, *in* P-60050
2,7-Dihydroxy-1,5,6-trimethoxyphenanthrene, *in* P-60050
7,9-Dihydroxy-2,3,4-trimethoxyphenanthrene, *in* P-70035
1-(2,5-Dihydroxy-3,4,6-trimethoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80050
2,8-Dihydroxy-3,9,10-trimethoxypterocarpan, *in* P-80054
1,8-Dihydroxy-2,3,6-trimethoxyxanthone, *in* P-70036
3,6-Dihydroxy-1,2,3-trimethoxyxanthone, *in* P-70036
3,8-Dihydroxy-1,2,4-trimethoxyxanthone, *in* P-60051
6,8-Dihydroxy-1,2,5-trimethoxyxanthone, *in* P-60052
1-(5,7-Dihydroxy-2,2,6-trimethyl-2*H*-1-benzopyran-8-yl)-2-methyl-1-propanone, D-70348
3,23-Dihydroxy-4,4,17-trimethylcholesta-7,14,24-trien-26-oic acid, *see* M-70012
4-(2,4-Dihydroxy-2,6,6-trimethylcyclohexylidene)-3-buten-2-one, *see* G-70028
7-[[5-(3,6-Dihydroxy-2,2,6-trimethylcyclohexyl)-3-methyl-2-pentyl]oxy]-2*H*-1-benzopyran-2-one, *see* K-80012
7-(10,11-Dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl)coumarin, *see* K-80004
7-[(10,11-Dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl)oxy]-2*H*-1-benzopyran-2-one, *see* K-80004
5,8-Dihydroxy-2,3,6-trimethyl-1,4-naphthalenedione, *see* D-60380
5,8-Dihydroxy-2,3,6-trimethyl-1,4-naphthoquinone, D-60380

3β,12β-Dihydroxy-4,4,14α-trimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, *in* L-60037
1-(5,7-Dihydroxy-2,2,6-trimethyl-2*H*-1-*benzopyran*-8-*yl*)-2-*methyl*-1-*butanone*, 9*CI*, *in* D-70348
3,15-Dihydroxy-7,11,23-trioxo-8,20-lanostadien-26-oic acid, D-80390
7β,15α-Dihydroxy-3,11,23-trioxo-8,20(22)*E*-lanostadien-26-oic acid, *in* T-70254
3β,7β-Dihydroxy-11,15,23-trioxo-8,20(22)*E*-lanostadien-26-oic acid, *in* T-70254
3β,28-Dihydroxy-7,11,15-trioxo-25,26,27-trisnor-8-lanosten-24-oic acid, *in* L-60036
3β,12β-Dihydroxy-7,11,15-trioxo-25,26,27-trisnor-8-lanosten-24-oic acid, *in* L-60037
2,10-Dihydroxy-11,12,13-trisnor-6-eremophilen-8-one, D-80391
2,3-Dihydroxytropone, *see* D-80307
2,4-Dihydroxytropone, *see* D-80308
2,5-Dihydroxytropone, *see* D-80309
2,6-Dihydroxytropone, *see* D-80308
2,7-Dihydroxytropone, *see* D-60314
2,7-Dihydroxytropone, *see* D-80307
3,5-Dihydroxytyrosyl-α,β-didehydro-3,5-dihydroxy-*N*-[2-(3,4,5-trihydroxyphenyl)ethenyl]tyrosinamide, *see* T-70336
1,11-Dihydroxy-6-undecanone, D-80392
2,3-Dihydroxy-12,20(30)-ursadien-28-oic acid, D-60381
3,19-Dihydroxy-12-ursene-23,28-dioic acid, D-80393
3,19-Dihydroxy-12-ursene-24,28-dioic acid, D-60382
1,3-Dihydroxy-12-ursen-28-oic acid, D-60383
2,3-Dihydroxy-12-ursen-28-oic acid, D-70349
3,19-Dihydroxy-12-ursen-28-oic acid, D-70350
4,6-Dihydroxy-5-vinylbenzofuran, D-70352
1,2-Dihydroxy-9*H*-xanthen-9-one, *see* D-70353
1,2-Dihydroxyxanthone, D-70353
Dihydroyashabushiketol, *in* D-70481
11α,13-Dihydroyomogin, *in* Y-70001
11α,13-Dihydrozaluzanin *C*, *in* Z-60001
11β,13-Dihydrozaluzanin *C*, *in* Z-60001
Di-2-imidazolylmethane, *see* M-70064
Di-1*H*-imidazol-2-ylmethanone, D-70354
2,2′-Diiminazole, *see* B-60107
2,4-Diimino-5,5-dimethyl-1-imidazolinyloxy, *see* P-70110
Di-2-indenyl sulfide, D-80394
Diindolo[3,2-*a*:3′,2′-*c*]carbazole, D-60384
Di-3-indolylcarbenium, *see* U-80033
1,2-Di-2-indolylethylene, D-80395
Di-3-indolylmethane, *see* M-80078
9,10-Diiodoanthracene, D-70355
2,3-Diiodobenzoic acid, D-80396
2,6-Diiodobenzoic acid, D-70356
1,4-Diiodobicyclo[2.2.2]octane, D-80397
1,3-Diiodobicyclo[1.1.1]pentane, D-70357
2,2′-Diiodo-1,1′-binaphthalene, *see* D-60385
4,4′-Diiodo-1,1′-binaphthalene, *see* D-60386
2,2′-Diiodo-1,1′-binaphthyl, D-60385
4,4′-Diiodo-1,1′-binaphthyl, D-60386
1,4-Diiodocubane, *see* D-70359
1,3-Diiodo-2,2-diazidopropane, D-60387
β,β′-Diiododiethyl ether, *see* O-60096
1,2-Diiodo-3,3-difluorocyclopropene, *see* D-80160
1,2-Diiodo-3,5-dinitrobenzene, D-80398
1,2-Diiodo-4,5-dinitrobenzene, D-80399
1,3-Diiodo-4,6-dinitrobenzene, D-80400
2,2′-Diiodo-4,5′-dinitrobiphenyl, D-80401
2,2′-Diiodo-5,5′-dinitrobiphenyl, D-80402
2,2′-Diiodo-6,6′-dinitrobiphenyl, D-80403
4,4′-Diiodo-3,3′-dinitrobiphenyl, D-80404
1,12-Diiodododecane, D-80405
1,3-Diiodo-2-(iodomethyl)propane, D-70358
1,4-Diiodopentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, D-70359
1,2-Diiodoperfluoroethane, *see* T-80050
2,7-Diiodophenanthrene, D-70360
3,6-Diiodophenanthrene, D-70361
sym-Diiodotetrafluoroethane, *see* T-80050
2,4-Diiodothiazole, D-60388
2,5-Diiodothiazole, D-60389
3,6-Diisobutylpiperazinedione, *see* B-60171
▷ 1,4-Diisocyanatocubane, D-80406
1,3-Diisocyanatocyclopentane, D-60390
▷ 1,4-Diisocyanatopentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, *see* D-80406
2,2′-Diisocyano-1,1′-binaphthalene, *see* D-60391
2,2′-Diisocyano-1,1′-binaphthyl, D-60391
Diisocyanogen, D-70362
3′,5′-Diisopentenyl-2′,4,4′-trihydroxychalcone, *see* D-60310
Diisoprene, *see* I-70087
2,3-Diisopropoxycyclopropenone, *in* D-70290
Diisopropylcyanamide, D-60392
3,4-Diisopropyl-2,5-dimethylhexane, D-60393
1,2:4,5-Di-*O*-isopropylidene-*myo*-inositol, *in* I-80015
6,8′;7,3′-Diligustide, *see* R-60009
6,6′;7,3*a*′-Diligustilide, D-70363
Dilophic acid, D-60394
Dilophus enone, D-80407
Dilophus ether, D-80408
▷ Dimazine, *see* D-70416
DIMBOA, *see* D-10388
1,3-Dimercaptobutane, *see* B-60339
2,2-Dimercaptobutane, *see* B-60340
1,4-Dimercapto-2-butene, *see* B-70292
1,4-Dimercapto-2-butyne, *see* B-70308
1,1-Dimercaptocyclobutane, *see* C-70215
1,3-Dimercaptocyclobutane, *see* C-60184
3,4-Dimercapto-3-cyclobutene-1,2-dithione, D-70364
▷ 1,1-Dimercaptocyclohexane, *see* C-60209
1,2-Dimercaptocyclohexane, *see* C-70225
1,1-Dimercaptocyclopentane, *see* C-60222
1,5-Dimercapto-3,3-dimethylpentane, *see* D-70427
1,3-Dimercapto-2,2-dimethylpropane, *see* D-70433
4,5-Dimercapto-1,3-dithiole-2-thione, D-80409
2-(4,5-Dimercapto-1,3-dithiol-2-ylidene)-4,5-dimercapto-1,3-dithiole, *see* T-70130
1,7-Dimercaptoheptane, *see* H-70023
(Dimercaptomethylene)malonic acid, *see* D-60395
(Dimercaptomethylene)malononitrile, *in* D-60395
(Dimercaptomethylene)propanedioic acid, D-60395
2,4-Dimercapto-6-methylpyrimidine, *see* M-70128
1,2-Dimercaptonaphthalene, *see* N-70002
1,8-Dimercaptonaphthalene, *see* N-70003
2,3-Dimercaptonaphthalene, *see* N-70004
4,6-Dimercapto-*m*-phenylenediamine, *see* D-70037
2,3-Dimercapto-*p*-phenylenediamine, *see* D-60030
2,3-Dimercapto-*p*-phenylenediamine, *see* D-70036
2,5-Dimercapto-*p*-phenylenediamine, *see* D-70035
2,2-Dimercaptopropane, *see* P-60175
2,3-Dimercapto-2-propene-1-thione, D-80410
3,6-Dimercaptopyridazine, *see* M-80028
2,3-Dimercaptopyridine, *see* P-60218
2,4-Dimercaptopyridine, *see* M-80029
2,4-Dimercaptopyridine, *see* P-60219
2,5-Dimercaptopyridine, *see* P-60220
3,4-Dimercaptopyridine, *see* P-60221
3,5-Dimercaptopyridine, *see* P-60222
2,5-Dimercapto-*p*-xylene, *see* D-60406
1,6:13,18-Dimethano[24]annulene, *see* T-80241
1,6:7,12-Dimethano[14]annulene, *see* B-60165
13,19:14,18-Dimethenoanthra[1,2-*a*]benzo[*o*]pentaphene, D-60396
3,4-Dimethoxbenzocyclobutene-1,2-dione, *in* D-80274
2,3-Dimethoxyaniline, *in* A-70089
▷ 3,4-Dimethoxyaniline, *in* A-70090
2,3-Dimethoxybenzaldehyde, *in* D-70285
2,3-Dimethoxybenzenamine, *in* A-70089
▷ 3,4-Dimethoxybenzenamine, *in* A-70090
2,5-Dimethoxybenzeneacetaldehyde, *in* D-60370
3,4-Dimethoxybenzeneacetaldehyde, *in* D-60371
4,5-Dimethoxy-1,3-benzenedicarboxylic acid, *in* D-60307
3,6-Dimethoxy-1,2-benzenediol, *in* B-60014
3,5-Dimethoxybenzocyclobutene-1,2-dione, *in* D-80275
3,6-Dimethoxybenzocyclobutene-1,2-dione, *in* D-80276
4,5-Dimethoxybenzocyclobutene-1,2-dione, *in* D-80277
3,6-Dimethoxybenzocyclobuten-1-one, *in* D-80278
4,5-Dimethoxybenzocyclobuten-1-one, *in* D-80279
4,6-Dimethoxybenzocyclobuten-1-one, *in* D-80280
5,6-Dimethoxybenzocyclobuten-1-one, *in* D-80281
3-(4,7-Dimethoxy-1,3-benzodioxol-5-yl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, *see* F-80006
5-(5,6-Dimethoxy-2-benzofuranyl)-1,3-benzenediol, *in* M-60146
3,9-Dimethoxy-6*H*-benzofuro[3,2-*c*][1]benzopyran, *in* D-80376
▷ 6,7-Dimethoxy-2*H*-1-benzopyran-2-one, *in* D-84287
3,6-Dimethoxy-1,2-benzoquinone, *in* D-60309
3,4-Dimethoxybenzyl isothiocyanate, D-80411
7,7′-Dimethoxy-[6,8′-bi-2*H*-benzopyran]-2,2′-dione, *in* B-70093
7,7′-Dimethoxy-8,8′-bi[2*H*-1-benzopyran-2-one], *see* J-80008
7,7′-Dimethoxy-6,8′-bicoumarin, *in* B-70093
7,7′-Dimethoxy-8,8′-bicoumarin, *see* J-80008
2,5-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-one, *in* D-80278
3,4-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-one, *in* D-80279
4,5-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-one, *in* D-80281
3,4′-Dimethoxybiphenyl, *in* B-80106
1,2-Dimethoxybiphenylene, *in* B-80116
1,5-Dimethoxybiphenylene, *in* B-80117
2,3-Dimethoxybiphenylene, *in* B-80119
2,6-Dimethoxybiphenylene, *in* B-80120
2,7-Dimethoxybiphenylene, *in* B-80121
3,5-Dimethoxy-4-biphenylol, *in* B-80129
2,2′-Dimethoxy-3,3′-bipyridine, *in* D-80287
3,3′-Dimethoxy-2,2′-bipyridine, *in* D-80290
4,4′-Dimethoxy-2,2′-bipyridine, *in* D-80294
5,5′-Dimethoxy-3,3′-bipyridine, *in* D-80298
6,6′-Dimethoxy-2,2′-bipyridine, *in* D-80299
6,6′-Dimethoxy-3,3′-bipyridine, *in* D-80300
4,4-Dimethoxybutanenitrile, *in* O-80068
1,1-Dimethoxy-2-butanol, *in* H-70112
1,1-Dimethoxy-2-butanone, *in* O-80067
4,4-Dimethoxybutylamine, *in* A-80064
Dimethoxycarbene, *in* D-80412
▷ 6,7-Dimethoxycoumarin, *in* D-84287
2,7-Dimethoxycycloheptene, *in* C-80179
5,6-Dimethoxy-1,3-cyclohexadiene, D-60397
3,6-Dimethoxycyclohexene, *in* C-80181
4,4-Dimethoxycyclohexene, *in* C-60211
Dimethoxycyclopropenone, *in* D-70290
1,1-Dimethoxy-3-decene, *in* D-70016
3,3-Dimethoxy-3*H*-diazirine, D-80412
2,6-Dimethoxy-3,5-dimethylbenzoic acid, *in* D-70293
6,7-Dimethoxy-2,2-dimethyl-2*H*-1-benzopyran, D-70365
6,7-Dimethoxy-2,2-dimethyl-3-chromene, *see* D-70365
5,7-Dimethoxy-α,α-dimethyl-2-oxo-2*H*-1-benzopyran-8-propanoic acid, *see* M-70158
5,5-Dimethoxy-3,3-dimethyl-1-pentyne, *in* D-80467

1,2-Dimethoxy-4,5-dinitrobenzene, *in* D-70449
1,5-Dimethoxy-2,4-dinitrobenzene, *in* D-80491
2,3-Dimethoxy-2,3-diphenylbutane, *in* D-80505
5,7-Dimethoxy-3′,4′-diprenyloxyisoflavone, *in* T-80109
3,3′-Dimethoxy-5,5′-di-2-propenyl[1,1′-biphenyl]-2,2′-diol, 9Cl, *see* D-80023
2,5-Dimethoxy-3-hexene, *in* H-80083
5,6-Dimethoxyindole, *in* D-70307
4′,7-Dimethoxyisoflavone, *in* D-80323
5,5′-Dimethoxylariciresinol, *in* L-70019
5,6-Dimethoxy-3-(4-methoxybenzyl)phthalide, D-60398
5,6-Dimethoxy-3-[(4-methoxyphenyl)methyl]-1(3*H*)-isobenzofuranone, *see* D-60398
2,6-Dimethoxy-4-(2-methoxyphenyl)phenol, *in* B-80128
9,10-Dimethoxy-2-methyl-1,4-anthraquinone, D-80413
2-(Dimethoxymethyl)benzenemethanol, *in* H-60171
α-(Dimethoxymethyl)benzenemethanol, *in* H-60210
4,5-Dimethoxy-2-methylbenzoic acid, *in* D-80339
4,7-Dimethoxy-5-methyl-2*H*-1-benzopyran-2-one, *in* D-60348
2,3-Dimethoxy-5-methyl-1,4-benzoquinone, *in* D-70320
2-(Dimethoxymethyl)benzyl alcohol, *in* H-60171
4,7-Dimethoxy-5-methylcoumarin, *in* D-60348
1,1-Dimethoxy-3-methylenecyclohexane, *in* M-80081
3′,5-Dimethoxy-3,4-methylenedioxybibenzyl, *in* T-60102
6,7-Dimethoxy-3′,4′-methylenedioxyflavanone, *in* T-70106
6,7-Dimethoxy-3′,4′-methylenedioxyisoflavanone, *in* T-80102
2′,7-Dimethoxy-4′,5′-methylenedioxyisoflavone, *in* T-80107
3′,4′-Dimethoxy-6,7-methylenedioxyisoflavone, *in* T-80111
3′,4′-Dimethoxy-7,8-methylenedioxyisoflavone, *in* T-70112
4′,5-Dimethoxy-6,7-methylenedioxyisoflavone, *in* D-80341
5,7-Dimethoxy-3′,4′-methylenedioxyisoflavone, *in* T-80109
6,7-Dimethoxy-3′,4′-methylenedioxyisoflavone, *in* T-80111
2,3-Dimethoxy-6,7-methylenedioxynaphthazarin, *in* H-60065
4,5-Dimethoxy-4′,5′-methylenedioxypolemannone, *in* P-60166
2,3-Dimethoxy-8,9-methylenedioxypterocarpan, *in* T-80117
3,4-Dimethoxy-8,9-methylenedioxypterocarpan, *in* T-80119
▷ 4,9-Dimethoxy-7-methyl-5*H*-furo[3,2-*g*][1]benzopyran-5-one, *see* K-60010
2-(Dimethoxymethyl)-1-naphthaldehyde, *in* N-60001
2-(Dimethoxymethyl)-1-naphthalenecarboxaldehyde, *in* N-60001
5,6-Dimethoxy-2-methyl-1,4-naphthoquinone, *in* D-60351
5,7-Dimethoxy-6-methylphthalide, *in* D-60349
1-(Dimethoxymethyl)-2,3,5,6-tetrakis(methylene)-7-oxabicyclo[2.2.1]heptane, D-60399
1,1-Dimethoxy-2(methylthio)ethane, *in* M-80017
2,4-Dimethoxy-6-methyl-1,3,5-triazine, *in* M-60132
4,5-Dimethoxy-1-naphthol, *in* N-60005
4,8-Dimethoxy-1-naphthol, *in* N-60005
1,4-Dimethoxy-2-naphthylamine, *in* A-80114
2,6-Dimethoxy-1-naphthylamine, *in* A-80112
2,7-Dimethoxy-1-naphthylamine, *in* A-80113
3,4-Dimethoxy-1-naphthylamine, *in* A-80117
3,4-Dimethoxy-2-naphthylamine, *in* A-80116
4,8-Dimethoxy-1-naphthylamine, *in* A-80119
5,6-Dimethoxy-1-naphthylamine, *in* A-80121
5,6-Dimethoxy-2-naphthylamine, *in* A-80124
6,7-Dimethoxy-1-naphthylamine, *in* A-80122
6,7-Dimethoxy-2-naphthylamine, *in* A-80123
2′,3′-Dimethoxy-6′-nitroacetophenone, *in* D-60357
2′,5′-Dimethoxy-4′-nitroacetophenone, *in* D-70322
3′,6′-Dimethoxy-2′-nitroacetophenone, *in* D-60358
4′,5′-Dimethoxy-2′-nitroacetophenone, *in* D-60359
4,5-Dimethoxy-2-nitrobenzoic acid, *in* D-60360
1,2-Dimethoxy-4-nitronaphthalene, *in* N-80053
1,4-Dimethoxy-2-nitronaphthalene, *in* N-80050
1,5-Dimethoxy-4-nitronaphthalene, *in* N-80054
2,3-Dimethoxy-6-nitronaphthalene, *in* N-80056
2,6-Dimethoxy-1-nitronaphthalene, *in* N-80048
4,6-Dimethoxy-1-nitronaphthalene, *in* N-80055
1,1-Dimethoxy-3-nitropropane, *in* N-60037
6,7-Dimethoxy-8-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-2*H*-1-benzopyran-2-one, *see* O-70044
5,5-Dimethoxy-2-pentanone, *in* O-60083
6,12-Dimethoxy-1,7-perylenedione, *in* D-80354
6,7-Dimethoxy-1,12-perylenedione, *in* D-80354
4,5-Dimethoxyphenanthrene, *in* P-70048
1,5-Dimethoxy-2,7-phenanthrenediol, *in* T-80114
3,4-Dimethoxy-2,7-phenanthrenediol, *in* T-80115
5,7-Dimethoxy-2,3-phenanthrenediol, *in* T-60120
5,7-Dimethoxy-2,6-phenanthrenediol, *in* T-80115
3,7-Dimethoxy-2-phenanthrenol, *in* T-60339
2,6-Dimethoxy-5*H*-phenanthro-[4,5-*bcd*]pyran-7-ol, *see* A-70077
1,2-Dimethoxy-3*H*-phenoxazin-3-one, *in* T-60353
2,5-Dimethoxyphenylacetaldehyde, *in* D-60370
3,4-Dimethoxyphenylacetaldehyde, *in* D-60371
1-(3,4-Dimethoxyphenyl)-2,3-bis(hydroxymethyl)-6,7-methylenedioxynaphthalene, D-80414
7-(2,4-Dimethoxyphenyl)-3,4-dihydro-5-hydroxy-10-(3-hydroxy-3-methylbutyl)-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, D-80415
7-(3,4-Dimethoxyphenyl)-3,4-dihydro-5-hydroxy-10-(3-hydroxy-3-methylbutyl)-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,6-*b*′]dipyran-6-one, D-80416
2-(3,4-Dimethoxyphenyl)-5,7-dihydroxy-6,8-dimethoxy-4*H*-1-benzopyran-4-one, *see* D-60376
2,2-Dimethoxy-1-phenylethanol, *in* H-60210
6-[2-(3,4-Dimethoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one, *in* H-70122
4-[4-(3,4-Dimethoxyphenyl)-1*H*,3*H*-furo[3,4-*c*]furan-1-yl]-2-methoxyphenol, *see* P-60141
3-(2,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* D-80366
4-[(3,4-Dimethoxyphenyl)methyl]dihydro-3-[(4-hydroxy-3-methoxyphenyl)methyl]-2(3*H*)-furanone, *see* A-70249
1,3-Dimethoxy-1-phenylpropane, *in* P-80122
3,4-Dimethoxyphthalaldehydic acid, *in* F-60070
5,6-Dimethoxyphthalaldehydic acid, *in* F-60073
5,7-Dimethoxyphthalide, *in* D-60339
12,13-Dimethoxy-8,11,13-podocarpatriene-3,7-dione, *in* D-80374
▷ 3,3-Dimethoxypropene, *in* P-70119
2-(3,3-Dimethoxypropyl)furan, *in* F-80089
3,9-Dimethoxypterocarpene, *in* D-80376
2,3-Dimethoxypyridine, *in* H-60223
2,4-Dimethoxypyridine, *in* H-60224
2,6-Dimethoxypyridine, *in* H-60226
3,4-Dimethoxypyridine, *in* H-60227
4,6-Dimethoxy-2(1*H*)-pyridinone, *in* D-70341
2,3-Dimethoxyquinoxaline, *in* D-60279
5,8-Dimethoxyquinoxaline, *in* Q-60002
6,7-Dimethoxyquinoxaline, *in* Q-60009
3β,21α-Dimethoxy-14-serratene, *in* S-80027
3β,21β-Dimethoxy-14-serratene, *in* S-80027
2,4-Dimethoxystyrene, *in* V-70010
6-(3,4-Dimethoxystyryl)-4-methoxy-2-pyrone, *in* H-70122
3,6-Dimethoxy-1,2,4,5-tetrazine, *in* D-70268
16,17-Dimethoxytricyclo[12.3.1.1^{2,6}]nonadeca-1(18),2,4,6(19),14,16-hexaene-3,9,15-triol, *see* M-70162
24,24-Dimethoxy-25,26,27-trisnor-3-cycloartanol, *in* H-60232
4,6-Dimethoxy-5-vinylbenzofuran, *in* D-70352
2,3-Dimethylacrolein, *see* M-80056
3,3-Dimethylacrolein, *see* M-70055
β,β-Dimethylacrylalkannin, *in* S-70038
β,β-Dimethylacrylshikonin, *in* S-70038
1,3-Dimethyladamantane, D-70366
3,7-Dimethyladenine, D-60400
3,9-Dimethyladenine, D-80417
8-Dimethylally-7-hydroxy-6-methylcoumarin, *see* C-60026
α,α-Dimethylallylcyclolobin, *in* U-80002
5′-(1,1-Dimethylallyl)-3′,7-dihydroxy-2′,4′-dimethoxyisoflavan, *see* U-80002
3-(1,1-Dimethylallyl)-6,7-dimethoxycoumarin, *see* R-80016
3-(1,1-Dimethylallyl)-7,8-dimethoxycoumarin, *see* D-80470
3-(1,1-Dimethylallyl)-8-hydroxy-7-methoxycoumarin, *in* D-80470
3-(1,1-Dimethylallyl)-7-hydroxy-6-(3-methyl-2-butenyl)coumarin, *see* G-60037
8-(3,3-Dimethylallyl)-5-methoxy-3,4′,7-trihydroxyflavan, *in* T-60125
3-(1,1-Dimethylallyl)scopoletin, *in* R-80016
8-(3,3-Dimethylallyl)-2′,4′,5,7-tetrahydroxyisoflavanone, *see* K-80010
2-(Dimethylallyl)trihydroxypterocarpan, *see* G-80028
4-(Dimethylallyl)trihydroxypterocarpan, *see* G-80027
3′-(γ,γ-Dimethylallyl)wighteone, *see* T-80290
2-(Dimethylamino)benzaldehyde, D-60401
N-[4-[2-(6-Dimethylaminobenzofuranyl)phenyl]]-maleimide, *see* D-60170
4-Dimethylamino-1,2,3-benzotriazine, *in* A-60092
6-(Dimethylamino)-3,3-bis[4-(dimethylamino)phenyl]-1(3*H*)-isobenzofuranone, *see* C-70202
1-(Dimethylamino)-γ-carboline, *in* A-70114
2-Dimethylamino-3,3-dimethylazirine, D-60402
8-(Dimethylamino)guanosine, *in* A-70150
8-(Dimethylamino)inosine, *in* A-70198
(Dimethylamino)methanesulfonic acid, *in* A-60215
Dimethyl 4-amino-5-methoxyphthalate, *in* A-70152
[[[(Dimethylamino)methylene]amino]methylene]dimethylammonium(1+), *see* G-80032
1-Dimethylamino-4-nitro-1,3-butadiene, D-70367
N-[4-[[4-(Dimethylamino)phenyl]imino]-2,5-cyclohexadien-1-ylidene]-*N*-methylmethanaminium, *see* B-60110
2-(Dimethylamino)purine, *in* A-60243
8-(Dimethylamino)purine, *in* A-60244
5-Dimethylamino-1*H*-tetrazole, *in* A-70202

2-Dimethylamino-6-(trihydroxypropyl)-4(3*H*)-pteridinone, *see* E-60070
10,10-Dimethyl-9(10*H*)-anthracenone, D-60403
10,10-Dimethylanthrone, *see* D-60403
3,3-Dimethylaspartic acid, *see* A-60147
N-(7,7-Dimethyl-3-azabicyclo[4.1.0]hepta-1,3,5-trien-4-yl)benzamide, D-70368
1,6-Dimethyl-5-azauracil, *in* M-60132
3,6-Dimethyl-5-azauracil, *in* M-60132
N,N-Dimethylazidochloromethylenimin-ium(1+), D-70369
1,6-Dimethylazulene, D-60404
4,7-Di-*O*-methylbellidin, *in* P-60052
▷ 7,12-Dimethylbenz[*a*]anthracene, D-60405
▷ 9,10-Dimethyl-1,2-benzanthracene (obsol.), *see* D-60405
α,2-Dimethylbenzeneacetic acid, *see* M-60113
α,4-Dimethylbenzeneacetic acid, *see* M-60114
2,5-Dimethyl-1,4-benzenedithiol, D-60406
3,6-Dimethyl-1,2,4,5-benzenetetracarboxylic acid, D-60407
2,3-Dimethyl-1,4-benzodioxin, D-70370
3,3-Dimethyl-2(3*H*)-benzofuranone, D-80418
7,8-Dimethylbenzo[*no*]naphtho[2,1,8,7-*ghij*]pleiadene, D-80419
2,2-Dimethyl-2*H*-1-benzopyran-6-carboxylic acid, D-60408
2,5-Dimethyl-4*H*-1-benzopyran-4-one, D-70371
3-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid, D-50601
3-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid, D-70372
2,2-Dimethyl-2*H*-1-benzothiopyran, D-70373
7,7-Dimethylbicyclo[4.1.0]hept-3-ene, D-60409
1,5-Dimethylbicyclo[3.3.0]octa-3,6-diene-2,8-dione, *see* D-70199
4,4-Dimethylbicyclo[3.2.1]octane-2,3-dione, D-60410
3,3-Dimethylbicyclo[2.2.2]octan-2-one, D-60411
3,3-Dimethylbicyclo[2.2.2]oct-5-en-2-one, D-60412
3,3′-Dimethyl-2,2′-biindazole, D-80421
5,5′-Dimethyl-2,2′-biindazole, D-80422
7,7′-Dimethyl-2,2′-biindazole, D-80423
Dimethylbiochanin *B*, *see* D-80323
1,4-Dimethylbiphenylene, D-80424
1,5-Dimethylbiphenylene, D-80425
1,8-Dimethylbiphenylene, D-80426
2,3-Dimethylbiphenylene, D-80427
2,6-Dimethylbiphenylene, D-80428
2,7-Dimethylbiphenylene, D-80429
2,2′-Dimethyl-4,4′-biquinoline, D-60413
2,5-Dimethyl-3,4-bis(1-methylethyl)hexane, *see* D-60393
1,4-Dimethyl-2,5-bis(methylthio)benzene, *in* D-60406
2,2′-Dimethyl-3,3′-bithiophene, D-80430
3,3′-Dimethyl-2,2′-bithiophene, D-80431
3,4′-Dimethyl-2,2′-bithiophene, D-80432
3,5-Dimethyl-2,3′-bithiophene, D-80433
4,4′-Dimethyl-2,2′-bithiophene, D-80434
4,4′-Dimethyl-3,3′-bithiophene, D-80435
5,5′-Dimethyl-2,2′-bithiophene, D-80436
5,5′-Dimethyl-3,3′-bithiophene, D-80437
5,5′-(2,3-Dimethyl-1,4-butanediyl)bis-1,3-benzodioxole, *see* A-70270
2,3-Dimethyl-3-butenoic acid, D-80438
2,3-Dimethyl-3-buten-1-ol, D-80439
1,1′-(2,2-Dimethyl-3-butenylidene)bisbenzene, *see* D-60418
3,3-Dimethyl-1-butynylbenzene, *see* D-60441
β,γ-Dimethylbutyrolactone, *see* D-80191
N,N-Dimethylcarbamohydroxamic acid, D-60414
1,2-Dimethylcarbazole, D-70374
1,3-Dimethylcarbazole, D-70375
1,4-Dimethylcarbazole, D-70376
1,5-Dimethylcarbazole, D-70377
1,6-Dimethylcarbazole, D-70378
1,7-Dimethylcarbazole, D-70379
1,8-Dimethylcarbazole, D-70380
2,3-Dimethylcarbazole, D-70381
2,4-Dimethylcarbazole, D-70382
2,5-Dimethylcarbazole, D-70383
2,7-Dimethylcarbazole, D-70384
3,4-Dimethylcarbazole, D-70385
3,5-Dimethylcarbazole, D-70386
3,6-Dimethylcarbazole, D-70387
4,5-Dimethylcarbazole, D-70388
1,2-Dimethyl-9*H*-carbazole-3,4,6-triol, *see* T-70253
24,24-Dimethyl-3-cholestanol, D-70389
27,27-Dimethyl-25-cholestene-1β,3β,5α-triol, *see* N-80085
2,2-Dimethylchroman, *see* D-80184
2,2-Dimethyl-6-chromancarboxaldehyde, *see* D-80185
2,2-Dimethyl-6-chromancarboxylic acid, *see* D-80186
2,2-Dimethylchromene-6-propenoic acid, *see* D-50601
2,5-Dimethylchromone, *see* D-70371
▷ 4,6-Dimethylcoumalin, *see* D-70435
Dimethyl cyanocarbonimidate, *see* D-70390
Dimethyl *N*-cyanoimidocarbonate, D-70390
2,3-Dimethyl-2-cyclobuten-1-one, D-60415
4,14-Dimethyl-9,19-cycloergost-20-en-3β-ol, *see* C-70218
2,7-Dimethyl-2,4,6-cycloheptatrien-1-one, D-70391
2,2-Dimethyl-5-cycloheptene-1,3-dione, D-60416
3,3-Dimethyl-1,4-cyclohexadiene, D-80440
4,4-Dimethyl-2,5-cyclohexadien-1-one, D-80441
6,6-Dimethyl-2,4-cyclohexadien-1-one, D-80442
2,2-Dimethyl-1,3-cyclohexanedione, D-80443
5,5-Dimethyl-2-cyclohexene-1,4-dione, D-70392
2,2-Dimethyl-1,3-cyclopentanedione, D-70393
4,4-Dimethyl-1,3-cyclopentanedione, D-70394
2,2-Dimethyl-4-cyclopentene-1,3-dione, D-70395
2,2-Dimethylcyclopropanecarboxylic acid, D-80444
2,2-Dimethylcyclopropanemethanol, D-70396
2,3-Dimethylcyclopropanol, D-70397
3,3-Dimethyl-1-cyclopropene-1-carboxylic acid, D-60417
4′,7-Di-*O*-methyldaidzein, *in* D-80323
4,8-Dimethyl-3*E*,8*E*-decadien-10-olide, *see* S-70084
Dimethyldehydrodieugenol, *in* D-80023
Dimethyl dicarbonate, *in* D-70111
2,3-Dimethyl-3,4-dihydro-2*H*-pyran, D-70398
1,3-Dimethyl-2,9-dioxabicyclo[3.3.1]nonane, D-80445
▷ 8,16-Dimethyl-1,9-dioxacyclohexadeca-3,11-diene-2,5,10,13-tetrone, *see* P-70167
Dimethyldioxirane, D-70399
3,3-Dimethyl-1,2-dioxolane, D-80446
2,2-Dimethyl-1,3-dioxolane-4-carboxaldehyde, D-70400
1-(2,2-Dimethyl-1,3-dioxolan-4-yl)ethanone, *see* A-70042
3,3′-Dimethyl-1,1′-diphenyl[$\Delta^{4,4'}$-bi-2-pyrazoline]-5,5′-dione, *see* P-70153
2,2-Dimethyl-4,4-diphenyl-3-butenal, D-70401
3,3-Dimethyl-4,4-diphenyl-1-butene, D-60418
2,2-Dimethyl-4,4-diphenyl-3-butenoic acid, D-70402
2,5-Dimethyl-3,4-diphenyl-2,4-cyclopentadien-1-one, D-70403
2,5-Dimethyl-3,4-diphenyl-2,4-hexadiene, D-60419
3,3-Dimethyl-5,5-diphenyl-4-pentenoic acid, D-60420
3,5-Dimethyl-2,6-diphenylpyridine, D-80447
▷ *N,N′*-Dimethyl-*N,N′*-diphenylurea, *in* D-70499
2,3-Dimethyl-1,4-dipiperonylbutane, *see* A-70270
9,18-Dimethyl-2,11-diselena[3.3]metacyclophane, D-70404
2,5-Dimethyl-1,4-dithiane-2,5-diol, D-60421
2-(4,6-Dimethyl-5*H*-1,3-dithiolo[4,5-*c*]pyrrol-2-ylidene)-5*H*-1,3-dithiolo[4,5-*c*]pyrrole, *see* B-80092
2,3-Dimethylenebicyclo[2.2.1]heptane, D-70405
2,3-Dimethylenebicyclo[2.2.3]nonane, D-70406
2,6-Dimethylenebicyclo[3.3.1]nonane, D-80448
7,8-Dimethylenebicyclo[2.2.2]octa-2,5-diene, D-70407
2,3-Dimethylenebicyclo[2.2.2]octane, D-70408
Dimethylenebicyclo[1.1.1]pentanone, D-60422
Dimethylenebutanedioic acid, D-70409
5,6-Dimethylene-1,3-cyclohexadiene, D-70410
1,2-Dimethylenecyclohexane, *see* B-60166
1,3-Dimethylenecyclohexane, *see* B-60167
1,4-Dimethylenecyclohexane, *see* B-60168
1,2-Dimethylenecyclopentane, *see* B-60169
1,2-Dimethylenecyclopentane, *see* B-60170
3,4;3′,4′-Dimethylenedioxybibenzyl, *in* T-60101
Dimethylenediurea, *see* T-70098
2,3-Dimethylenenorbornane, *see* D-70405
3,4-Dimethyleneoxolane, *see* T-70046
Dimethylenesuccinic acid, *see* D-70409
3,4-Dimethylenetetrahydrofuran, *see* T-70046
6,6′-(1,2-Dimethyl-1,2-ethanediyl)bis[1-phenazinecarboxylic acid], D-70411
3-(1,1-Dimethylethoxy)dihydro-2,5-furandione, *in* D-80211
2-(1,1-Dimethylethyl)-1-butene-1-thione, *see* D-60114
3-(1,1-Dimethylethyl)-2-cyclobuten-1-one, *see* B-80283
1-(1,1-Dimethylethyl)-1,3-cyclohexadiene, *see* B-70296
1-(1,1-Dimethylethyl)cyclohexene, *see* B-60341
3-(1,1-Dimethylethyl)cyclohexene, *see* B-60342
4-(1,1-Dimethylethyl)cyclohexene, *see* B-60343
3-(1,1-Dimethylethyl)-2-cyclohexen-1-one, *see* B-70297
1-(1,1-Dimethylethyl)-1,2-cyclooctadiene, *see* B-60344
6-(1,1-Dimethylethyl)cyclopenta[*c*]pyran, *see* B-80284
1-(1,1-Dimethylethyl)cyclopentene, *see* B-70298
3-(1,1-Dimethylethyl)cyclopentene, *see* B-70299
4-(1,1-Dimethylethyl)cyclopentene, *see* B-70300
(1,1-Dimethylethyl)cyclopropane, *see* B-80285
3-(1,1-Dimethylethyl)-1,4,2-dioxazol-5-one, *see* B-80286
4-(1,1-Dimethylethyl)-3*H*-1,2,3,5-dithiadiazol-3-yl, *see* B-70302
5-(1,1-Dimethylethyl)-1,3,2,4-dithiadiazol-2-yl, *see* B-70303
3-(1,1-Dimethylethyl)-4-hydroxybenzaldehyde, *see* B-70304
4-(1,1-Dimethylethyl)-2-hydroxycyclopentanecarboxylic acid, *see* H-70113
▷ Dimethylethylideneurea, *in* I-70005
▷ 2-[(1,1-Dimethylethyl)imino]tetrahydro-3-(1-methylethyl)-5-phenyl-4*H*-1,3,5-thiadiazin-4-one, *see* B-80276
1-(1,1-Dimethylethyl)-2-iodobenzene, *see* B-60346
1-(1,1-Dimethylethyl)-3-iodobenzene, *see* B-60347
1-(1,1-Dimethylethyl)-4-iodobenzene, *see* B-60348
3-(1,1-Dimethylethyl)-6-oxabicyclo[3.1.0]hexane, *see* B-70294
4-(1,1-Dimethylethyl)-2(3*H*)-oxazolethione, *see* B-80288
3-(1,1-Dimethylethyl)-2,2,4,5,5-pentamethyl-3-hexene, *see* B-60350
2-(1,1-Dimethylethyl)pentanedioic acid, *see* B-80289

2-(1,1-Dimethylethyl)phenanthrene, *see* B-70305
3-(1,1-Dimethylethyl)phenanthrene, *see* B-70306
9-(1,1-Dimethylethyl)phenanthrene, *see* B-70307
3(5)-(1,1-Dimethylethyl)pyrazole, *see* B-80291
4-(1,1-Dimethylethyl)pyrazole, *see* B-80292
2,5-Dimethyl-3-furancarboxaldehyde, D-70412
4,5-Dimethyl-2-furancarboxylic acid, D-70413
4,5-Dimethyl-2,3-furandicarboxylic acid, D-80449
3,4-Dimethyl-2(5*H*)-furanone, D-60423
4,4-Dimethylglutaraldehydic acid, *see* D-60434
4,4-Dimethylglutaraldehydonitrile, *in* D-60434
4,4-Dimethyl-6-heptenoic acid, D-80450
4′-(3,6-Dimethyl-2-heptenyloxy-5-hydroxy-3′,7-dimethoxyflavanone, *in* T-70105
4-(1,5-Dimethyl-1,3-hexadienyl)-1-isocyano-1-methylcyclohexane, *see* I-60091
4-(1,5-Dimethyl-1,4-hexadienyl)-1-methyl-7-oxabicyclo[4.1.0]heptane, *see* E-60009
2,5-Dimethyl-1,3,5-hexatriene, D-60424
2,2-Dimethyl-4-hexen-3-one, D-70414
2,2-Dimethyl-5-hexen-3-one, D-60425
2-(1,5-Dimethyl-4-hexenyl)-*p*-cresol, *see* E-60004
9-(1,5-Dimethyl-4-hexenyl)-2,6-dimethyl-2,5-cyclononadiene-1-carboxylic acid, *see* D-60394
5-(1,5-Dimethyl-4-hexenyl)-3-hydroxy-2-methyl-2,5-cyclohexadiene-1,4-dione, *see* I-70075
1-(1,5-Dimethyl-4-hexenyl)-4-methylenebicyclo[3.1.0]hexane, *see* S-70037
2-(1,5-Dimethyl-4-hexenyl)-4-methylphenol, *see* E-60004
2-(1,5-Dimethyl-4-hexenyl)-5-methylphenol, *see* C-70208
5-(1,5-Dimethyl-4-hexenyl)-2-methylphenol, *see* X-70001
5,5-Dimethyl-2-hexynedioic acid, D-70415
▷ 1,1-Dimethylhydrazine, D-70416
5,5-Dimethyl-1-hydroxy-1-cyclopenten-3-one, *see* D-70394
1,4-Dimethyl-4-[4-hydroxy-2-(hydroxymethyl)-1-methyl-2-cyclopentenyl]-2-cyclohexen-1-ol, D-70417
O,N-Dimethylhydroxylamine, D-70418
1,2-Dimethylidenecyclohexane, *see* B-60166
1,3-Dimethylidenecyclohexane, *see* B-60167
1,4-Dimethylidenecyclohexane, *see* B-60168
1,2-Dimethylidenecyclopentane, *see* B-60169
1,2-Dimethylidenecyclopentane, *see* B-60170
▷ 1,3-Dimethylimidazolidinone, *in* I-70005
1,3-Dimethyl-1*H*-imidazolium(1+), D-80451
2,2-Dimethyl-1-indanone, *see* D-60227
1,6-Dimethyl-1*H*-indole, *in* M-60088
1,3-Dimethyl-1*H*-indole-2-carboxaldehyde, *in* M-70090
1,4-Di-*O*-methyl-*myo*-inositol, D-80452
3,4-Dimethylmaleimide, *see* D-80474
5,13-Dimethyl[2.2]metacyclophane, D-60426
▷ *N,N*-Dimethylmethanamine *N*-oxide, *see* T-60354
N,N-Dimethylmethaneselenoamide, *in* M-70035
N,1-Dimethyl-4-(methylamino)-1*H*-imidazole-5-carboxamide, *see* C-60003
2,2-Dimethyl-3-methylenebicyclo[2.2.2]octane, D-60427
4,4-Dimethyl-5-methylene-γ-butyrolactone, *see* D-70197
4-(2,2-Dimethyl-6-methylenecyclohexyl)-3-buten-2-one, *see* I-70058
3-[2-(2,2-Dimethyl-6-methylenecyclohexyl)ethyl]furan, *see* P-60015
2,2-Dimethyl-4-methylene-1,3-dioxolane, D-70419
5,5-Dimethyl-4-methylene-1,2-dioxolan-3-one, D-60428
1,3-Dimethyl-2-methyleneimidazolidine, D-70420
6,10-Dimethyl-2-(1-methylethenyl)spiro[4.5]dec-6-ene, *see* P-70114
1,7-Dimethyl-4-(1-methylethyl)bicyclo[3.2.1]oct-6-ene-6,8-dicarboxaldehyde, *see* H-60016
2,10-Dimethyl-7-(1-methylethyl)spiro[4.5]dec-1-en-6-ol, *see* I-80079
1,3-Dimethyl-8-(1-methylethyl)tricyclo[4.4.0.0^{2,7}]dec-3-ene, *see* C-70197
1,5-Dimethyl-8-(5-methyl-1-methylene-4-hexenyl)-1,5-cyclodecadiene, D-80453
6,6-Dimethyl-2-(2-methyl-1-oxopropyl)-4-cyclohexene-1,3-dione, *see* X-70002
1,2-Dimethyl-2-(4-methylphenyl)cyclopentanemethanol, *see* T-70202
2,6-Dimethyl-3-morpholinone, D-80454
8,8-Dimethyl-1,4,5(8*H*)-naphthalenetrione, D-70421
2,3-Dimethylnaphthazarin, *see* D-60317
2,2-Dimethyl-1-(1-naphthyl)propane, *see* D-60446
2,2-Dimethyl-1-(2-naphthyl)propane, *see* D-60447
▷ Dimethylnitramine, *see* N-80045
N,N-Dimethyl-4-nitro-1,3-butadien-1-amine, *see* D-70367
4,4-Dimethyl-6-nitro-5-hexenenitrile, *in* D-60429
4,4-Dimethyl-6-nitro-5-hexenoic acid, D-60429
α-(4,8-Dimethyl-3,7-nonadienyl)-1,2-dihydro-α,4-dimethylfuro[2,3-*c*]quinoline-2-methanol 5-oxide, *see* A-60313
α-(4,8-Dimethyl-3,7-nonadienyl)-2-formyl-3-(hydroxymethyl)-2-cyclopentene-1-acetaldehyde, *see* F-70038
4-[3-(4,8-Dimethyl-3,7-nonadienyl)-3-methyloxiranyl]-2-butanone, *see* E-80047
α-(4,8-Dimethyl-3,7-nonadienyl)tetrahydro-5-methoxy-α,5-dimethyl-2-furanmethanol, *see* M-80047
4,8-Dimethyl-1,3,7-nonatriene, D-50644
3-(4,8-Dimethyl-2,4,6-nonatrienyl)furan, *see* D-80022
2,6-Dimethyl-2,7-octadiene-1,6-diol, D-80456
2,6-Dimethyl-3,7-octadiene-2,6-diol, D-70422
3,7-Dimethyl-2,5-octadiene-1,7-diol, D-80457
3-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxybenzoic acid, D-70423
2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone, D-80458
1-[2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyphenyl]ethanone, *see* D-80458
7-(3,7-Dimethyl-2,6-octadienyl)oxy-2*H*-1-benzopyran-2-one, *see* A-80187
1-[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,5,6-tetrahydroxyphenyl]-3-(4-hydroxyphenyl)-1-propanone,9CI, D-80459
3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzophenone, D-80460
[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-trihydroxyphenyl]phenylmethanone, *see* D-80460
3,7-Dimethyl-6-octenal, D-60430
3,7-Dimethyl-6-octen-4-olide, *see* E-70004
4,6-Dimethyl-4-octen-3-one, D-70424
Dimethyloldihydroxyethyleneurea, *see* D-80301
6,6-Dimethyl-3-oxabicyclo[3.1.0]hexan-2-one, D-70425
2,5-Dimethyl-4-oxazolecarboxylic acid, D-80461
3,5-Dimethyl-2-oxazolidinone, *in* M-60107
4,4-Dimethyl-2-oxazoline, *see* D-70198
β,β-Dimethyloxiraneethanol, D-60431
2,3-Dimethyloxiranemethanol, D-80462
3,3-Dimethyloxiranemethanol, D-70426
2-(3,3-Dimethyloxiranyl)-4-ethenyl-3,4-dihydro-2-hydroxy-4,10-dimethyl-2*H*,5*H*-pyrano[3,2-*c*][1]benzopyran-5-one, *see* E-60045
4-(3,3-Dimethyloxiranyl)methoxy-7*H*-1,3-dioxolo[4,5-*f*][1]benzopyran-7-one, *see* D-80463
7-(3,3-Dimethyloxiranyl)methoxy-5,6-methylenedioxycoumarin, D-80463
7-[[5-(3,3-Dimethyloxiranyl)-3-methyl-2-pentenyl]oxy]-2*H*-1-benzopyran-2-one, *in* A-80187
13-(3,3-Dimethyloxiranyl)-3,7,11-trimethyl-2,6,10-tridecatrienal, *see* E-80045
2,6-Dimethyl-8-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-2,6-octadienal, *see* U-80001
3-[1-(1,1-Dimethyl-3-oxobutyl)imidazol-4-yl]-2-propenoic acid, *in* U-70005
4-(3,5-Dimethyl-4-oxo-2,5-cyclohexadien-1-ylidene)-2,6-dimethyl-2,5-cyclohexadien-1-one, *see* T-80140
4,4-Dimethyl-3-oxo-1-cyclopentene-1-carboxaldehyde, D-60432
4-(1,5-Dimethyl-3-oxo-1-hexenyl)-1-cyclohexene-1-carboxylic acid, *see* O-80066
4,4-Dimethyl-17-oxo-18-nor-16-oxaandrostane-8-carboxaldehyde, *see* O-60094
2,2-Dimethyl-4-oxo-1-pentanal, D-80464
3,3-Dimethyl-4-oxopentanoic acid, D-60433
4,4-Dimethyl-5-oxopentanoic acid, D-60434
2,2-Dimethyl-4-oxothiochromane, *see* D-70193
6,12-Dimethyl-2-pentadecanone, D-80465
2,4-Dimethyl-1,3-pentanediol, D-80466
3,3-Dimethyl-1,5-pentanedithiol, D-70427
3,4-Dimethylpentanoic acid, D-60435
4,4-Dimethylpentanoic acid, D-70428
3,4-Dimethyl-1-pentanol, D-60436
3,3-Dimethyl-4-pentenoic acid, D-60437
3,3-Dimethyl-4-penten-2-one, D-70429
7-(1,3-Dimethyl-1-pentenyl)-7,8-dihydro-4,8-dihydroxy-3,8-dimethyl-2*H*,5*H*-pyrano[4,3-*b*]pyran-2-one, *see* N-70029
▷ 3,4-Dimethyl-5-pentylidene-2(5*H*)-furanone, D-70430
3,3-Dimethyl-4-pentynal, D-80467
4,4-Dimethyl-2-pentyne, D-60438
4,4-Dimethyl-1-pentyn-3-ol, D-80468
4,5-Dimethylphenanthrene, D-60439
2,2-Dimethyl-3-phenyl-2*H*-azirine, D-60440
3,3-Dimethyl-1-phenyl-1-butyne, D-60441
4,5-Dimethyl-2-phenyl-1,3-dioxol-1-ium, D-70431
2,5-Dimethyl-3-(2-phenylethenyl)pyrazine, D-60442
2-(2,4-Dimethylphenyl)-5-hydroxy-6-methoxybenzofuran, *in* S-60002
4,4-Dimethyl-2-phenyl-4*H*-imidazole, D-70432
2,4-Dimethyl-5-phenyloxazole, D-80469
2,2-Dimethyl-1-phenylpropane, *see* D-60445
2,2-Dimethyl-1-phenyl-1-propanone, D-60443
4,6-Dimethyl-2-phenylpyrimidine, D-60444
1,2-Dimethyl-5-phenylpyrrolidine, *in* M-80147
N,S-Dimethyl-*S*-phenylsulfoximine, *in* M-80148
2,2-Dimethyl-1,3-propanedithiol, D-70433
6-(1,1-Dimethyl-2-propenyl)-2,3-dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, *see* C-60031
6-(1,1-Dimethyl-2-propenyl)-5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* D-80472
3-(1,1-Dimethyl-2-propenyl)-7,8-dimethoxy-2*H*-1-benzopyran-2-one, D-80470
3-(1,1-Dimethyl-2-propenyl)-6,7-dimethoxy-2*H*-1-benzopyran-2-one, *see* R-80016
6-(1,1-Dimethyl-2-propenyl)-8*H*-1,3-dioxolo[4,5-*h*][1]benzopyran-8-one, *see* R-70015
3-[5-(1,1-Dimethyl-2-propenyl)-3-hydroxy-2,4-dimethoxyphenyl]-3,4-dihydro-2*H*-1-benzopyran-7-ol, *see* U-80002

10-(1,1-Dimethyl-2-propenyl)-5-hydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, *see* N-80079
3-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, *in* D-80470
3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, *see* G-60037
3-(1,1-Dimethyl-2-propenyl)-4-hydroxy-6-phenyl-2*H*-pyran-2-one, D-70434
4-(1,1-Dimethyl-2-propenyl)-2-(3-methyl-2-butenyl)phenol, D-80471
4-(1,1-Dimethylpropenyl)-7,8-methylenedioxycoumarin, *see* R-70015
6-(1,1-Dimethyl-2-propenyl)-4′,5,7-trihydroxyisoflavone, D-80472
2-(1,1-Dimethyl-2-propenyl)-1,5,6-trihydroxy-3-methoxy-9*H*-xanthen-9-one, *see* C-80163
4-(1,1-Dimethyl-2-propenyl)-1,2,5-trihydroxy-9H-xanthen-9-one, *see* G-80020
Dimethyl-*β*-propriothetin, *see* C-80024
(2,2-Dimethylpropyl)benzene, D-60445
▷ Dimethylpropyleneurea, *in* T-60088
1-(2,2-Dimethylpropyl)naphthalene, D-60446
2-(2,2-Dimethylpropyl)naphthalene, D-60447
7,8-(2,2-Dimethylpyrano)-3,4′-dihydroxy-5-methoxyflavan, *in* D-60448
▷ 4,6-Dimethyl-2*H*-pyran-2-one, D-70435
7,8-(2,2-Dimethylpyrano)-3,4′,5-trihydroxyflavan, D-60448
7,6-(2,2-Dimethylpyrano)-3,4′,5-trihydroxyflavone, D-60449
2-(3,5-Dimethyl-1*H*-pyrazol-1-yl)pyridine, D-80473
4,5-Dimethylpyrimidine, D-70436
4,6-Dimethyl-2(1*H*)-pyrimidinethione, D-60450
Dimethyl pyrocarbonate, *in* D-70111
▷ 4,6-Dimethyl-*α*-pyrone, *see* D-70435
1,5-Dimethyl-1*H*-pyrrole-2-carboxaldehyde, *in* M-70129
3,4-Dimethyl-1*H*-pyrrole-2,5-dione, D-80474
2,5-Dimethylpyrrolidine, D-70437
5,5-Dimethyl-1-pyrroline, *see* D-60229
Dimethylpyruvic acid, *see* M-80129
3,3-Dimethyl-2,4(1*H*,3*H*)-quinolinedione, D-60451
3,5-Di-*O*-methylsenecioodontol, *in* S-60022
2,5-Dimethyl-3-styrylpyrazine, *see* D-60442
Dimethylsulfonium 9-fluorenylide, D-80475
Dimethyl tartrate, *in* T-70005
4′,7-Di-*O*-methyltectorigenin, *in* T-80112
2,2-Dimethyltetralone, *see* D-60228
2,2-Dimethylthiazolidine, *see* D-80194
2,2-Dimethyl-2*H*-thiochromene, *see* D-70373
4,6-Dimethyl-2-thio-2,3-dihydropyrimidine, *see* D-60450
2,5-Dimethyl-3-thiophenecarboxaldehyde, D-70438
3,5-Dimethyl-2-thiophenecarboxaldehyde, D-70439
1,2-Dimethyl-9*H*-thioxanthen-9-one, *see* D-70440
1,3-Dimethyl-9*H*-thioxanthen-9-one, *see* D-70441
1,4-Dimethyl-9*H*-thioxanthen-9-one, *see* D-70442
2,3-Dimethyl-9*H*-thioxanthen-9-one, *see* D-70443
2,4-Dimethyl-9*H*-thioxanthen-9-one, *see* D-70444
3,4-Dimethyl-9*H*-thioxanthen-9-one, *see* D-70445
1,2-Dimethylthioxanthone, D-70440
1,3-Dimethylthioxanthone, D-70441
1,4-Dimethylthioxanthone, D-70442
2,3-Dimethylthioxanthone, D-70443
2,4-Dimethylthioxanthone, D-70444
3,4-Dimethylthioxanthone, D-70445
5,8-Dimethyltocol, *see* T-80200
5,5-Dimethyl-Δ^1-1,2,4-triazolin-3-one, *see* D-80196
3,5-Dimethyl-2,4,6-tribromobenzaldehyde, D-80476
3,5-Dimethyl-2,4,6-trichlorobenzaldehyde, D-80477
1,3-Dimethyltricyclo[3.3.1.1^{3,7}]decane, *see* D-70366
6,13-Dimethyltricyclo[9.3.1.1^{4,8}]hexadeca-1(15),4,6,8(16),11,13-hexaene, *see* D-60426
10,10-Dimethyltricyclo[7.1.1.0^{2,7}]undec-2-en-4-one, *see* T-80242
2,3-Dimethyl-5-(2,6,10-trimethylundecyl)thiophene, D-70446
3,5-Dimethyl-2,4,6-triphenylpyridine, D-80478
2,7-Dimethyltropone, *see* D-70391
β,*β*-Dimethyltyrosine, *see* A-60198
4,4-Dimethylvaleric acid, *see* D-70428
γ,*δ*-Dimethyl-*δ*-valerolactone, *see* T-70059
2,7-Dimethyl-9*H*-xanthen-9-one, *see* D-60453
2,7-Dimethylxanthone, D-60453
1,1-Di-4-morpholinylethene, D-70447
Dimyristyl ketone, *see* N-80066
1,2-Di-2-naphthalenyl-1,2-ethanediol, D-80479
1,2,3:6,7,8-Di(1′,8′-naphth)[10]annulene, *see* C-60187
Dinaphtho[1,8-*ab*,1′,8′-*fg*]cyclodecene, *see* C-60187
Dinaphtho[2,3-*a*:2′,3′-*e*]cyclooctene, *see* C-60216
7*H*,9*H*,16*H*,18*H*-Dinaphtho[1,8-*cd*:1′,8′-*ij*][1,7]dithiacyclododecin, D-70448
Dinaphtho[7′:1′-1:13][1″:7″-6:8]peropyrene, *see* D-60072
Dinaphtho[1,2,3-*cd*:1′,2′,3′-*lm*]perylene, *see* B-60038
Dinaphtho[1,2,3-*cd*:3′,2′,1′-*lm*]perylene, *see* A-60279
Dinaphtho[2,1,8,7-*ghij*:2′,2′,8′,7′-*nopq*]pleiadene, *see* C-80134
Dinaphtho[1,2-*b*:1′,2′-*d*]thiophene, D-80480
Dinaphtho[1,2-*b*:2′,1′-*d*]thiophene, D-80481
Dinaphtho[1,2-*b*:2′,3′-*d*]thiophene, D-80482
Dinaphtho[2,1-*b*:1′,2′-*d*]thiophene, D-80483
Dinaphtho[2,1-*b*:2′,3′-*d*]thiophene, D-80484
Dinaphtho[2,3-*b*:2′,3′-*d*]thiophene, D-80485
2,2-Di-(*α*-naphthyl)acetaldehyde, *see* D-80486
2,2-Di-(*β*-naphthyl)acetaldehyde, *see* D-80487
1,3-Di-(1-naphthyl)benzene, D-60454
1,3-Di(2-naphthyl)benzene, D-60455
2,2-Di-(1-naphthyl)ethanal, D-80486
2,2-Di-(2-naphthyl)ethanal, D-80487
7,11:20,24-Dinitrilodibenzo[*b*,*m*][1,4,12,15]tetraazacyclodocosine, D-60456
1,1-Dinitroacetone, *see* D-70454
2,2-Dinitroadamantane, D-50699
2,4-Dinitroadamantane, D-80489
2,6-Dinitroadamantane, D-80490
3,5-Dinitrobenzamide, *in* D-60458
4,5-Dinitro-1,2-benzenediol, D-70449
▷ 4,6-Dinitro-1,3-benzenediol, D-80491
2,6-Dinitrobenzenemethanol, *see* D-60459
2,6-Dinitrobenzoic acid, D-60457
3,5-Dinitrobenzoic acid, D-60458
2,4-Dinitrobenzotrifluoride, *see* D-70456
3,5-Dinitrobenzotrifluoride, *see* D-70455
2,6-Dinitrobenzyl alcohol, D-60459
2,2′-Dinitrobiphenyl, D-60460
1,5-Dinitrobiphenylene, D-80492
2,6-Dinitrobiphenylene, D-80493
4,5-Dinitrocatechol, *see* D-70449
▷ 3,5-Dinitro-4-chlorobenzotrifluoride, *see* C-80053
1,2-Dinitrocyclohexene, D-70451
1,2-Dinitrocyclopropane, D-80494
1,12-Dinitrododecane, D-80495
4,5-Dinitroguaiacol, *in* D-70449
3,5-Dinitroisoxazole, D-70452
▷ 2,4-Dinitropentane, D-70453
1,1-Dinitro-2-propanone, D-70454
2,3-Dinitro-1*H*-pyrrole, D-60461
2,4-Dinitro-1*H*-pyrrole, D-60462
2,5-Dinitro-1*H*-pyrrole, D-60463
3,4-Dinitro-1*H*-pyrrole, D-60464
▷ 4,6-Dinitroresorcinol, *see* D-80491
▷ 2,6-Dinitrotoluene, *see* M-60061
2,2-Dinitrotricyclo[3.3.1.1^{3,7}]decane, *see* D-50699
2,4-Dinitrotricyclo[3.3.1.1^{3,7}]decane, *see* D-80489
2,6-Dinitrotricyclo[3.3.1.1^{3,7}]decane, *see* D-80490
1,3-Dinitro-5-(trifluoromethyl)benzene, D-70455
2,4-Dinitro-1-(trifluoromethyl)benzene, D-70456
4,5-Dinitroveratrole, *in* D-70449
▷ Dinopron *EM*, *in* D-60367
▷ Dinoprostone, *in* D-60367
24,25-Dinor-1,3,5(10)-lupatriene, D-80496
24,25-Dinor-1,3,5(10),12-oleanatetraene, D-80497
14,15-Dinor-13-oxo-7-labden-17-oic acid, D-70457
24,25-Dinor-1,3,5(10),12-ursatetraene, D-80498
Dioctadecylacetic acid, *see* O-70005
▷ 1,3-Diodo-2-methylenepropane, *see* I-60047
Diomelquinone *A*, *in* D-60351
Dioscin, *in* S-60045
3-epi-Diosgenin, *in* S-60045
▷ Diosgenin, *in* S-60045
Diospyroside, *in* D-84287
2,4-Dioxaadamantane, *see* D-80503
1,4-Dioxa-8-azaspiro[4.7]dodecane, *in* H-70047
1,4-Dioxa-9-azaspiro[4.7]dodecane, *in* H-70048
Dioxa-1,3-bishomopentaprismane, *see* D-70461
1,6-Dioxacyclodeca-3,8-diene, D-70458
1,7-Dioxa-4,10-diazacyclododecane, D-60465
5,12-Dioxa-7,14-diazapentacene, *see* T-60378
2*H*-1,5,2,4-Dioxadiazine-3,6(4*H*)dione, D-60466
4,9-Dioxa-1,6,11-dodecatriyne, D-80499
1,3-Dioxahexaaza-24-crown-8, *see* D-70460
1,13-Dioxa-4,7,10,16,20,24-hexaazacyclohexacosane, D-70459
1,13-Dioxa-4,7,10,16,19,22-hexaazacyclotetracosane, D-70460
11,12-Dioxahexacyclo[6.2.1.1^{3,6}.0^{2,7}.0^{4,10}.0^{5,9}]dodecane, D-70461
5,12-Dioxanaphthacene, *see* B-80026
1,4-Dioxane-2,6-dione, D-80500
2,2′-(1,3-Dioxan-2-ylidene)bispyridine, *in* D-70502
8,13-Dioxapentacyclo[6.5.0.0^{2,6}.0^{5,10}.0^{3,11}]-tridecane-9,12-dione, D-60467
Dioxapyrrolomycin, *see* P-70203
7,10-Dioxaspiro[5.4]deca-2,5-dien-4-one, *in* B-70044
1,6-Dioxaspiro[4,5]decane, D-80501
1,4-Dioxaspiro[4.5]decane-7-thiol, *in* M-70026
1,4-Dioxaspiro[4,5]dec-7-ene, *in* C-60211
2,6-Dioxaspiro[3.3]heptane, D-60468
3,9-Dioxaspiro[5.5]undecane, D-70462
5,12-Dioxatetracyclo[7.2.1.0^{4,11}.0^{6,10}]dodeca-2,7-diene, D-70463
1,3,2-Dioxathiane, D-80502
2,4-Dioxatricyclo[3.3.1.1^{3,7}]decane, D-80503
2*H*-1,5,2-Dioxazine-3,6(4*H*)-dione, D-70464
▷ 1,2-Dioxetane, D-60469
1,5-Dioxiranyl-1,2,3,4,5-pentanepentol, D-70465
3,23-Dioxo-8(14→13*R*)-abeo-17,13-friedo-9*β*-lanosta-7,14,24*E*-trien-26-oic acid, *see* I-60108
3,23-Dioxo-8(14→13*R*)-abeo-17,13-friedo-9*β*-lanosta-7,14(30),24*E*-trien-26-oic acid, *see* M-60011
2,2′-Dioxo-*N*,*N*′-bipyrrolidinyl, *see* B-70125
3,6-Dioxo-4,7,11,15-cembratetraen-10,20-olide, D-60470
3,4-Dioxo-1,5-cyclohexadiene-1-carboxylic acid, *see* B-70046

5,6-Dioxo-1,3-cyclohexadiene-1-carboxylic acid, *see* B-70045
2,5-Dioxo-3,6-cyclohexadiene-1,3-dicarboxylic acid, *see* B-70049
3,6-Dioxo-1,4-cyclohexadiene-1,2-dicarboxylic acid, *see* B-70047
3,6-Dioxo-1,4-cyclohexadiene-1,4-dicarboxylic acid, *see* B-70048
2,5-Dioxo-3,4-dimethyl-Δ^3-pyrroline, *see* D-80474
9,12-Dioxododecanoic acid, D-60471
1,1′-(1,2-Dioxo-1,2-ethanediyl)bis-1*H*-indole-2,3-dione, D-70466
1,2-Dioxolane, D-70467
1,3-Dioxolane-2,2-diacetic acid, *in* O-60084
1,3-Dioxolane-2-methanol, D-70468
3,23-Dioxo-7,24-lanostadien-26-oic acid, D-60472
3,23-Dioxo-7,25(27)-lanostadien-26-oic acid, *in* D-60472
1,3-Dioxole, D-60473
6*H*-1,3-Dioxolo[4,5-*g*][1]benzopyran-6-one, *see* M-70068
3,7-Dioxo-12-oleanen-28-oic acid, D-70469
3,5-Dioxo-1,2,4-oxadiazolidine, *see* O-70060
3,4-Dioxopyrrolizidine, *see* D-70260
4,5-Dioxo-4,5-seco-11(13)-eudesmen-12,8β-olide, *see* U-60001
2,4-Dioxo-1,2,3,4-tetrahydropyrimido[4,5-*b*]quinoline, *see* P-60245
1,3-Dioxototaryl methyl ether, *in* T-70204
4,5-Dioxo-1(10)-xanthen-12,8-olide, D-60474
▷ Dipentene, *in* I-70087
Diphenanthro[2,1-*b*:1′,2′-*d*]furan, D-70470
Diphenanthro[9,10-*b*:9′,10′-*d*]furan, D-70471
Diphenanthro[5,4,3-*abcd*:5′,4′,3′-*jklm*]perylene, *see* D-60072
Di-9-phenanthrylamine, D-70472
Diphenospiropyran, *see* S-70062
2,5-Diphenyladipic acid, *see* D-80510
3,4-Diphenyladipic acid, *see* D-80511
2,3-Diphenylallyl bromide, *see* B-70209
▷ Diphenylamine-2,2′-dicarboxylic acid, *see* I-60014
Diphenylamine-2,3′-dicarboxylic acid, *see* I-60015
Diphenylamine-2,4′-dicarboxylic acid, *see* I-60016
Diphenylamine-3,3′-dicarboxylic acid, *see* I-60017
Diphenylamine-4,4′-dicarboxylic acid, *see* I-60018
2,2-Diphenylaziridine, D-80504
α,α-Diphenylbenzeneacetaldehyde, *see* T-80359
7,7-Diphenylbenzo[*c*]fluorene, D-70473
1,3-Diphenylbenzo[*c*]thiophene, D-70474
1,1′-Diphenylbicyclohexyl, D-70475
1,1-Diphenyl-1,3-butadiene, D-70476
2,3-Diphenyl-2,3-butanediol, D-80505
2,3-Diphenylbutanoic acid, D-80506
2,3-Diphenyl-4-butanolide, *see* D-80202
4,4-Diphenyl-4-butanolide, *see* D-80203
1,3-Diphenyl-2-butanone, D-80507
2,3-Diphenyl-2-butenal, D-60475
2,4-Diphenyl-3-butyn-1-ol, D-80508
4,4-Diphenylbutyrolactone, *see* D-80203
α,α-Diphenyl-γ-butyrolactone, *see* D-80198
α,β-Diphenyl-γ-butyrolactone, *see* D-80199
α,γ-Diphenyl-γ-butyrolactone, *see* D-80200
β,β-Diphenyl-γ-butyrolactone, *see* D-80201
2,3-Diphenylcrotonaldehyde, *see* D-60475
3,3-Diphenylcyclobutanone, D-60476
1,2-Diphenyl-1,4-cyclohexadiene, D-60477
1,1-Diphenylcyclopropane, D-60478
1,2-Diphenyl-1,2-cyclopropanedicarboxylic acid, D-80509
Diphenylcyclopropenone anil, *see* D-70491
N-(2,3-Diphenyl-2-cyclopropen-1-ylidene)benzenamine, *see* D-70491
3,6-Diphenyl-2,5-diaza-1,4(2*H*,5*H*)-pentalenedione, *see* D-70204
1,2-Diphenyl-1,2-diazetidin-3-one, *in* D-70055
4,6-Diphenyl-1,2-dihydropyrimidine, *see* D-60235
2,5-Diphenyl-1,3-dioxol-1-ium, D-70478
2,11-Diphenyldipyrrolo[1,2-*a*:2′,1′-*c*]quinoxaline, D-70479
1,2-Diphenyl-1,2-ethanediamine, D-70480
α-(2,2-Diphenylethenyl)-α-phenylbenzeneacetaldehyde, *see* T-70148
Diphenyl ether 4-carboxylic acid, *see* P-80088
1,2-Diphenylethylenediamine, *see* D-70480
N,*N*′-Diphenylformamidine, D-60479
1,7-Diphenyl-3,5-heptanediol, D-70481
1,7-Diphenyl-1,3,5-heptanetriol, D-60480
7,7-Diphenyl[2.2.1]hericene, *see* D-70488
2,5-Diphenylhexanedioic acid, D-80510
3,4-Diphenylhexanedioic acid, D-80511
Diphenyl imidocarbonate, *in* C-70019
1,3-Diphenyl-1*H*-indene-2-carboxylic acid, D-60481
2,3-Diphenyl-1*H*-inden-1-one, D-70482
2,3-Diphenylindole, D-70483
2,3-Diphenylindone, *see* D-70482
Diphenylketazine, D-80512
Diphenylmethaneimine, D-60482
N,*N*′-Diphenylmethanimidamide, *see* D-60479
Diphenylmethanone-2-carboxylic acid, *see* B-80054
Diphenylmethanone-2,2′-dicarboxylic acid, *see* B-70041
Diphenylmethanone (diphenylmethylene)hydrazone, *see* D-80512
Diphenylmethylamine, *see* M-70060
Diphenylmethyl diselenide, *see* B-70141
N-(Diphenylmethylene)acetamide, *in* D-60482
7-(Diphenylmethylene)bicyclo[4.1.0]hepta-1,3,5-triene, *see* D-70484
1-(Diphenylmethylene)-1*H*-cyclopropabenzene, D-70484
1-(Diphenylmethylene)-1*H*-cyclopropa[*b*]naphthalene, D-70485
2,2-Diphenyl-4-methylene-1,3-dioxolane, D-70486
4-(Diphenylmethylene)-1(4*H*)-naphthalenone, D-70487
7-(Diphenylmethylene)-2,3,5,6-tetramethylenebicyclo[2.2.1]heptane, D-70488
1,1-Diphenylmethylenimine, *see* D-60482
Diphenylmethyl isocyanate, *see* I-80054
N-(Diphenylmethyl)-α-phenylbenzenemethanamine, *see* T-70150
1,8-Diphenylnaphthalene, D-60483
3,5-Diphenyl-1,2,4-oxadiazole, D-60484
2,4-Diphenyl-5-oxazolamine, *see* A-80070
2,5-Diphenyl-4-oxazolamine, *see* A-80069
4,5-Diphenyl-2-oxazolamine, *see* A-80068
3,4-Diphenyl-1,3-oxazolidin-2-one, *in* P-60126
3,4-Diphenyl-2-oxazolidinone, *in* P-60126
2,4-Diphenyl-2-oxazolin-5-one, *see* D-60485
2,4-Diphenyl-5(4*H*)-oxazolone, D-60485
2,7-Diphenyloxepin, D-60486
1,1-Diphenyl-1,3-pentadiene, D-70489
Diphenyl pentaketone, *see* D-60488
1,5-Diphenyl-1,3-pentanediol, D-70490
1,5-Diphenylpentanepentone, D-60488
1,5-Diphenyl-1,3,5-pentanetrione, D-60489
5,5-Diphenyl-4-pentenoic acid, D-80513
9,18-Diphenylphenanthro[9,10-*b*]triphenylene, D-60490
1,2-Diphenyl-3-(phenylimino)cyclopropene, D-70491
2,3-Diphenyl-1-(phenylmethylene)-1*H*-indene, *see* B-80059
(Diphenylpropadienylidene)propanedioic acid, D-70492
2,2-Diphenylpropanoic acid, D-70493
1,1-Diphenylpropene, D-60491
2,2-Diphenylpropiophenone, *see* T-60389
2,3-Diphenylpropiophenone, *see* T-60390
3,3-Diphenylpropiophenone, *see* T-60391
2,4-Diphenylpyrimidine, D-70494
4,5-Diphenylpyrimidine, D-70495
4,6-Diphenylpyrimidine, D-70496
3,4-Diphenyl-1,2,5-selenadiazole, D-70497
▷ Diphenylstyrylcarbinol, *see* T-70313
Diphenyl sulfide-2,2′-dicarboxylic acid, *see* T-70174
Diphenyl sulfide 4,4′-dicarboxylic acid, *see* T-70175
Diphenyltartaric acid, *see* D-80312
Diphenyl tartrate, *in* T-70005
2,5-Diphenyl-1,2,4,5-tetraazabicyclo[2.2.1]heptane, D-70498
9,18-Diphenyltetrabenz[*a*,*c*,*h*,*j*]anthracene, *see* D-60490
N,*N*′-Diphenyl-1,2,4-thiadiazole-3,5-diamine, *see* D-70048
2,2-Diphenyl-1,3,4-thiadiazoline, *see* D-60236
4,6-Diphenylthieno[2,3-*c*]furan, D-80514
2,6-Diphenyl-4*H*-thiopyran-4-one, D-60492
▷ *N*,*N*′-Diphenylurea, D-70499
▷ Diphosgene, *see* T-70223
▷ Diphosphopyridine nucleotide, *see* C-80145
▷ Diphyllin, D-60493
▷ Di-1-piperidinyl disulfide, *see* D-70523
1,1-Di-1-piperidinylethene, D-70500
2,4-Diprenylphenol, *see* B-80155
N,*N*′-Di-2-propenyl-1,2-hydrazinedicarbothioamide, *see* D-60026
▷ *N*,*N*-Di-2-propenyl-2-propen-1-amine, *see* T-70315
Di-2-propenyl tetrasulfide, D-80515
Dipropyl 4,4′-bipyridinium disulfonate, *see* B-70160
Dipteryxin, *in* P-70032
Dipteryxin/, *in* P-80043
Dipyridiniomethane, *see* M-70065
Di-2-pyridinylmethanone, *see* D-70502
Di-3-pyridinylmethanone, *see* D-70503
Di-4-pyridinylmethanone, *see* D-70504
N,*N*′-Di-2-pyridinyl-1,4-phthalazinediamine, *see* B-60172
Dipyrido[1,2-*a*:1′,2′-*c*]imidazol-10-ium(1+), D-70501
Dipyrido[1,2-*a*: 1′,2′-*c*]imidazolium-11-thiolate, D-80516
Dipyrido[1,2-*a*:1′,2′-*e*]-1,3,4,6-tetraazapentalene, *see* P-60234
Dipyrido[1,2-*b*:1′,2′-*e*][1,2,4,5]tetrazine, D-60494
6*H*-Dipyrido[1,2-*a*:2′,1′-*d*][1,3,5]triazin-5-ium, D-60495
▷ 2,3′-Dipyridyl, *see* B-60120
1,4-Di(2-pyridylamino)phthalazine, *see* B-60172
2,2′-Dipyridyl ether, *see* O-60098
2,3′-Dipyridyl ether, *see* O-60099
2,4′-Dipyridyl ether, *see* O-80099
3,3′-Dipyridyl ether, *see* O-60100
4,4′-Dipyridyl ether, *see* O-60101
Di-2-pyridyl ketone, D-70502
Di-3-pyridyl ketone, D-70503
Di-4-pyridyl ketone, D-70504
Di-2-pyridylmethane, D-60496
2,2′-Dipyridyl oxide, *see* O-60098
2,3′-Dipyridyl oxide, *see* O-60099
2,4′-Dipyridyl oxide, *see* O-80099
3,3′-Dipyridyl oxide, *see* O-60100
4,4′-Dipyridyl oxide, *see* O-60101
2,2′-Dipyridyl selenide, *see* S-80023
4,4′-Dipyridyl selenide, *see* S-80024
Di-2-pyridyl sulfite, D-60497
Disain, D-80517
Disalicylaldehyde, D-70505
1,2-Diselenete, D-60498
2-(1,3-Diselenol-2-ylidene)-1,3-diselenole, *see* B-70116
3′,4′-Disenecioyloxy-3′,4′-dihydroseselin, *in* K-70013
Disidein, D-60499
▷ Disnogamycin, D-70506
Disogluside, *in* S-60045
Dispiro[cyclopropane-1,5′-[3,8]dioxatricyclo[5.1.0.0^{2,4}]octane-6′,1″-cyclopropane], D-60500

Dispiro[2.0.2.4]dec-8-ene-7,10-dione, D-60501
Dispiro[tricyclo[3.3.1.1^{3,7}]decane-2,2′-oxirane-3,2″-tricyclo[3.3.1.1^{3,7}]decane], *see* B-70091
Distanol, *see* K-80006
Distichol, D-60502
▷ Distylin, *see* P-70027
Distyryl selenide, D-60503
2-(1,3-Ditellurol-2-ylidene)-1,3-tellurole, *see* B-70117
Ditetradecyl ketone, *see* N-80066
1,2-Dithiacyclodecane, *see* D-60507
1,2-Dithiacycloheptane, *see* D-70517
1,5-Dithiacyclononane, *see* D-70526
1,2-Dithiacyclooctane, *see* D-50815
9,10-Dithia-1,6-diazaanthracene, *see* D-70518
9,10-Dithia-1,7-diazaanthracene, *see* D-70520
9,10-Dithia-1,8-diazaanthracene, *see* D-70519
1,4-Dithiafulvalene, *see* C-60221
8,8-Dithiaheptafulvene, *see* C-70221
1,3-Dithiane-2-selone, D-70507
2-(1,3-Dithian-2-yl)pyridine, D-60504
3,6-Dithia-1,8-octanediol, *see* B-70145
3,6-Dithia-1,8-octanedithiol, *see* B-70150
2,11-Dithia[3.3]orthocyclophane, *see* T-80058
2,11-Dithia[3.3]paracyclophane, D-60505
2,18-Dithia[3.1.3.1]paracyclophane, D-80518
8,20-Dithiapentacyclo[20.2.2.2^{3,6}.2^{10,13}.2^{15,18}]dotriaconta-3,5,10,12,15,17,22,24,25,27,29,31-dodecaene, *see* D-80518
3,10-Dithiaperylene, *see* P-60072
1,6-Dithiapyrene, *see* B-60049
Dithiatopazine, D-70508
2,7-Dithiatricyclo[6.2.0.0^{3,6}]deca-1(8),3(6)-diene-4,5,9,10-tetrone, D-60506
3,10-Dithiatricyclo[10.2.2.2^{5,8}]octadeca-5,7,12,14,15,17-hexaene, *see* D-60505
2,2′-Dithiazolyl, *see* B-70166
2,4′-Dithiazolyl, *see* B-70167
2,5′-Dithiazolyl, *see* B-70168
4,4′-Dithiazolyl, *see* B-70169
4,5′-Dithiazolyl, *see* B-70170
5,5′-Dithiazolyl, *see* B-70171
1,2-Dithiecane, D-60507
Dithieno[2,3-*b*:2′,3′-*d*]pyridine, D-70509
Dithieno[2,3-*b*:3′,2′-*d*]pyridine, D-70510
Dithieno[2,3-*b*:3′,4′-*d*]pyridine, D-70511
Dithieno[3,2-*b*:2′,3′-*d*]pyridine, D-70512
Dithieno[3,2-*b*:3′,4′-*d*]pyridine, D-70513
Dithieno[3,4-*b*:2′,3′-*d*]pyridine, D-70514
Dithieno[3,4-*b*:3′2′-*d*]pyridine, D-70515
Dithieno[3,4-*b*:3′,4′-*d*]pyridine, D-70516
1,2-Dithiepane, D-70517
[1,4]Dithiino[2,3-*b*:6,5-*b*′]dipyridine, D-70519
1,4-Dithiino[2,3-*b*:5,6-*c*′]dipyridine, D-70518
1,4-Dithiino[2,3-*b*:6,5-*c*′]dipyridine, D-70520
[1,4]Dithiino[2,3-*b*]-1,4-dithiin, D-70521
Dithiobis(carbonylchloride), *see* B-80142
3,3′-Dithiobiscyclobutanol, *in* M-60019
N,N′-[Dithiobis[2,1-ethanediylimino(3-oxo-3,1-propanediyl)]]bis[2,4-dihydroxy-3,3-dimethylbutanamide], *see* P-80009
N,N′-[Dithiobis(ethyleneiminocarbonylethylene)]bis[2,4-dihydroxy-3,3-dimethylbutyramide], *see* P-80009
2,2′-Dithiobis-1*H*-isoindole-1,3(2*H*)-dione, D-70522
5,5′-Dithiobis[1-methylhistidine], *in* M-80025
Dithiobisphthalimide, D-60508
Dithiobisphthalimide, *see* D-70522
▷ 1,1′-Dithiobispiperidine, D-70523
1,1′-Dithiobis-2,5-pyrrolidinedione, D-70524
N,N′-Dithiobissuccinimide, *see* D-70524
2,2′-Dithiobisthiazole, *in* T-60200
N,N′-[Dithiobis(trimethylene)]bis[3-aminopropionamide], *see* H-60084
1,2-Dithiocane, D-50815
Dithiocarbazic acid, D-60509
Dithiocarbazinic acid, *see* D-60509
1,4-Dithiocyano-2-butene, D-60510
1,1-Dithiocyclopentane, *see* C-60222
N,N′-(Dithiodi-2,1-ethanediyl)bis[3-aminopropanamide], *see* A-60073
N,N′-(Dithiodi-2,1-ethanediyl)bis[3-bromo-4-hydroxy-α-(hydroxyimino)benzenepropanamide], *see* B-70130
N,N′-(Dithiodiethylene)bis[3-aminopropionamide], *see* A-60073
N,N′-(Dithiodi-3,1-propanediyl)bis[3-aminopropanamide], *see* H-60084
1,3-Dithiolane-2-selone, D-70525
2-(1,3-Dithiolo[4,8-*b*][1,4]-dithiin-2-ylidene)-1,3-dithiolo[4,5-*b*][1,4]dithiin, *see* B-70118
2-(1,3-Dithiol-2-ylidene)-1,3-dithiole, *see* B-70119
1,5-Dithionane, D-70526
1,4-Dithioniabicyclo[2.2.0]hexane, D-70527
▷ Dithiooxamide, *see* E-60041
Dithiosilvatin, D-60511
▷ Dithiothymine, *see* M-70127
2,6-Dithioxobenzo[1,2-*d*:4,5-*d*′]bis[1,3]dithiole-4,8-dione, D-60512
5,8-Dithioxo-1,6-tridecadiene-3,9,11-triyne, *see* T-80255
7,10-Dithioxo-1,8-tridecadiene-3,5,11-triyne, *see* T-80256
7,10-Dithioxo-1,3,8-tridecatriene-5,11-diyne, *see* T-80248
Di-*p*-toluoyl tartrate, *in* T-70005
▷ Diurea, *see* T-70097
Divaronic acid, D-70528
Divaroside, *in* C-70038
1,3-Divinyladamantane, D-70529
▷ Divinylethylene glycol, *see* H-70036
▷ 1,2-Divinylglycol, *see* H-70036
Divinylglyoxal, *see* H-60039
DMDHEU, *see* D-80301
▷ DMI, *in* I-70005
▷ DMPU, *in* T-60088
▷ 1,1*a*,2,2,3,3*a*,4,5,5,5*a*,5*b*,6-Dodecachlorocyclooctahydro-1,3,4-metheno-1*H*-cyclobuta[*cd*]pentalene, *see* D-70530
▷ Dodecachlorodihomocubane, *see* D-70530
▷ Dodecachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{5,8}]decane, D-70530
2,3-Dodecadien-1-ol, D-80520
2,6-Dodecadien-5-olide, *see* H-60025
Dodecafluorobicyclobutylidene, D-60513
Dodecahedranamine, *see* A-80071
Dodecahedrane, D-60514
Dodecahedranecarboxaldehyde, D-80521
Dodecahedranecarboxylic acid, D-80522
Dodecahedranemethanol, *see* H-80201
Dodecahedranol, D-80523
1,3,5,7,9,11-Dodecahexaene, D-70531
Dodecahydrocarbazole, D-70532
7,8,10,11,13,14,23,24,26,27,29,30-Dodecahydro-5,3,2[1′,2′]:16,21[1″,2″]dibenzenodibenzo[*l,z*][1,4,7,10,15,18,21,24]octaoxacyclooctacosin, *see* H-70085
Dodecahydro-6*H*,13*H*-5*a*,12*a*-epidithiopyrano[3,2-*b*]pyrano[2′,3′:6,7]oxepino[2,3-*f*]oxepin, *see* D-70508
Dodecahydro-2,6,3,5-ethanediylidenecyclobut[*jkl*]-*as*-indacene, *see* H-70013
Dodecahydropentaleno[1,6-*cd*]pentalene, *see* T-60035
1,2,2*a*,3,4,4*a*,5,7,8,9,10,10*a*-Dodecahydro-3,3,4*a*,7,10*a*-pentamethylpentaleno[1,6-*cd*]azulene, *see* L-60018
Dodecahydro-1,7*a*:2,3*b*:3*a*,5:6,7*b*-tetramethanodicyclobuta[*b,h*]biphenylene, *see* N-70070
Dodecahydro-3*a*,6,6,9*a*-tetramethylnaphtho[2,1-*b*]furan, D-70533
2,3,4,5,6,7,8,10,11,12,13,?-Dodecahydro-1,4:5,8:10,13-triethano-1*H*-tribenzo[*a,c,e*]cycloheptenylium(1+), D-80524
1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydro-1,4:5,8:9,12-triethanotriphenylene, D-80525
1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydrotriphenylene, D-60516
Dodecamethylene diiodide, *see* D-80405
2,6-Dodecanedione, D-70534
3,3′-(1,2-Dodecanediyl)bis[5-methoxy-6-methylphenol], *see* M-80002
4,7,10,15,18,21,24,27,30,33,36,39-Dodecaoxatricyclo[11.9.9.9^{2,12}]tetraconta-1,12-diene, D-70535
▷ 1-*O*-(1,3,5,7,9-Dodecapentaenyl)-*sn*-glycerol, *in* D-70536
3-(1,3,5,7,9-Dodecapentaenyloxy)-1,2-propanediol, D-70536
1-*O*-(4,6,8-Dodecatrienyl)glycerol, D-80526
3-(4,6,8-Dodecatrienyloxy)-1,2-propanediol, *see* D-80526
9-Dodecen-1-ol, D-70537
10-Dodecen-12-olide, *in* H-60126
5-Dodecen-7-yne, D-70538
2-Dodecyl-3-methylbutanedioic acid, D-80527
2-Dodecyl-3-methylsuccinic acid, *see* D-80527
11-Dodecyn-1-ol, D-70540
5-Dodecyn-1-ol, D-70539
3,7-Dolabelladiene-6,12-diol, D-70541
Dolastatin 10, D-70542
1(15)-Dolastene-4,8,9,14-tetrol, D-70543
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Dolichosterone, D-70544
Dolineone, D-80528
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7,8,9,10,24,25,27,28,30,31,33,34,36,37,39,40,54,55,56,57,71,72,74,75,77,78,80,1,83,84,86,87-Dotriacontahydro-1,93:4,6:11,13:16,18:19,22:42,45:46,48:51,53:58,60:63,65:66,69:89,92-dodecathenotetrabenzo[z,j_1,q_2,a_3][1,4,7,10,13,16,19,44,47,50,53,56,59,62,25,28,35,38,68,71,78,81]tetradecaoxaota D-80529
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6-Drimene-8,9,11-triol, D-70547
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9(11)-Drimen-8-ol, D-60520
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Eburicoic acid, E-80001
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Eccremocarpol A, E-80002
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Egonol 2-methylbutanoate, *in* E-70001
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(E)-ω-Hydroxyferulenol, *in* F-80007
2-Eicosanol, *see* I-80002
5,8,11,14,16-Eicosapentaenoic acid, E-80009
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6-Eicosyl-4-methyl-2*H*-pyran-2-one, *see* A-60291
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(−)-Epiafzelechin, *in* T-60104
Epialeuritolic acid, *in* H-80256
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Epicatechin, *in* P-70026
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7-Epicedronin, *in* C-70027
10-Epicumambranolide, *in* C-80164
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7-Epidebneyol, *in* D-70010
10-Epi-8-deoxycumambrin B, *in* C-80164
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11-Epidihydroridentin, *in* R-70007
3,6-Epidioxy-6-methoxy-4,16,18-eicosatrienoic acid, E-60007
3,6-Epidioxy-6-methoxy-4-octadecenoic acid, E-60008
9,10-Epidithio-9,10-dihydroanthracene, *see* D-70206
9′-Epiencecanescin, *in* E-70008
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1-Epierivanin, *in* E-70033
7-Epi-α-eudesmol, *in* E-80086
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1-Epi-α-gurjunene, *in* G-70034
22-Epihippurin 1, *in* E-80039
22-Epihippuristanol, *in* E-80039
13-Epihomoverrucosan-5β-ol, *in* H-80095
5-Epiilimaquinone, *in* I-80004
6-Epi-7-isocucurbic acid, *in* C-50302
1-Epiisoerivanin, *in* I-70066
2′-Epiisotriptiliocoumarin, *in* I-80096
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2-Epijatrogrossidione, *in* J-70002
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Epilophodione, *in* D-60470
1′-Epilycoserone, *in* L-70045
3-Epimesembryanthemoidigenic acid, *in* D-80347
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6-Epimonomelittoside, *in* M-70019
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4-Epineopulchellin, *in* N-70028
13-Epi-5β-neoverrucosanol, *in* N-70030
13-Epi-5β-neoverrucosanol, *in* N-80024
10-Epinidoresedic acid, *in* N-70035
6-Epiophiobolin *A*, *in* O-70040
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13-Episclareol, *in* S-70018
3-Episiaresinolic acid, *in* D-70327
Epispongiadiol, *in* D-70345
Epitaxifolin, *in* P-70027
12-Epiteupolin II, *in* T-70159
12-Epiteuscordonin, *in* T-80165
12-Epiteuscorodonin, *in* T-80165
22-Epitokorogenin, *in* S-60043
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4-Epivulgarin, *in* V-80013
3-Epizaluzanin *C*, *in* Z-60001
4β,15-Epoxy-9*E-millerenolide*, *in* M-60137
4β,15-Epoxy-9*Z-millerenolide*, *in* M-60137
12,16-Epoxy-8,11,13-abietatriene, *see* A-60008
1,2-Epoxyacenaphthene, *see* D-70170
1,2-Epoxyacenaphthylene, *see* D-70170
1β,10β-Epoxyachillin, *in* A-80033
6′,7′-Epoxyaurapten, *in* A-80187
2,3-Epoxy-7,10-bisaboladiene, E-60009
10,11-Epoxy-2,7(14)-bisaboladien-4-one, E-80014
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▷ 1,2-Epoxybutane, *see* E-70047
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2,3-Epoxybutyric acid, *see* M-80127
11,13-Epoxy-4-cadinen-15-oic acid, *in* H-80135
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7,8-Epoxy-2,11-cembradiene-4,6-diol, E-60010
3,4-Epoxy-7,11,15(17)-cembratrien-16,2-olide, *see* I-60106
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ent-3α,4α-Epoxy-13,15-clerodanediol, E-80017
ent-3α,4α-Epoxy-15-clerodanoic acid, E-80018
ent-4α,18-Epoxy-15-clerodanoic acid, *in* C-80142
ent-4β,18-Epoxy-15-clerodanoic acid, *in* C-80142
ent-4α,18-Epoxy-13-cleroden-15-oic acid, *in* C-80142
ent-4β,18-Epoxy-13-cleroden-15-oic acid, *in* C-80142
ent-3α,4α-Epoxy-13-cleroden-15,16-olide, E-80019
3′,6′-Epoxycycloauraptene, E-80020
3,6-Epoxy-1-cyclohexene, *see* O-70054
4,5-Epoxycyclohexene, *see* O-60047
20,24-Epoxy-9,19-cyclolanostane-3,16,25-triol, *see* Q-70011
1,2-Epoxy-5-cyclooctene, *see* O-70058
5,8-Epoxydaucane, E-80021
8α,9α-Epoxy-2α,4β,6α,10α-daucanetetrol, *see* L-60015
7,8-Epoxy-4,6,9-daucanetriol, E-80022
6,12-Epoxy-6*H*,12*H*-dibenzo[*b*,*f*][1,5]dioxocin, *see* D-70505
5,6-Epoxy-5,6-dihydro-12′-apo-β-carotene-3,12′-diol, *see* P-60065
5,6-Epoxy-5,6-dihydro-β,ε-carotene-3,3′-diol, *see* E-80011
▷ 5,6-Epoxy-5,6-dihydrochrysene, *see* C-70174
1,2-Epoxy-1,2-dihydrolycopene, *in* L-60041
5,6-Epoxy-5,6-dihydrolycopene, *in* L-60041
2,3-Epoxy-2,3-dihydro-1,4-naphthoquinone, E-70011
1,2-Epoxy-1,2-dihydrotriphenylene, *see* T-60385
12,16-Epoxy-11,14-dihydroxy-5,8,11,13-abietatetraen-7-one, E-60011
11,12-Epoxy-2,14-dihydroxy-5,8(17)-briaradien-18,7-olide, E-70012
24*R*,25-Epoxy-11β,23*S*-dihydroxydammar-13(17)-en-3-one, *see* A-70082
2,3-Epoxy-1,4-dihydroxy-7(11),8-eudesmadien-12,8-olide, E-60012
4,5-Epoxy-2,8-dihydroxy-1(10),11(13)-germacradien-12,6-olide, E-60013
9β,10β-Epoxy-1α,3β-dihydroxy-4*Z*-germacren-12,6α-olide, *in* D-80318
24,25-Epoxy-7,26-dihydroxy-8-lanosten-3-one, E-70013
2α,3α-Epoxy-1β,4α-dihydroxy-8β-methoxy-7(11)-eudesmen-12,8-olide, *in* E-60033
5,6-Epoxy-3,4-dihydroxy-2-methyl-2-cyclohexen-1-one, *see* T-70009
22,25-Epoxy-3β,17α-dihydroxy-11-oxo-7-lanosten-18,20*S*-olide, *see* D-70237
6α,7α-Epoxy-5α,20*R*-dihydroxy-1-oxo-22*R*,24*S*,25*R*-with-2-enolide, *see* I-60143
11,15-Epoxy-1,2-dihydroxy-3(20)-phytene, *see* E-80043
24*R*,25-Epoxy-11β,23*S*-dihydroxy-13(17)-protosten-3-one, *see* A-70082
6,11-Epoxy-6,12-dihydroxy-6,7-seco-8,11,13-abietatrien-7-al, E-60014
15,20-Epoxy-2α,3β-dihydroxy-14,15-seco-5,15,17(20)-pregnatrien-14-one, *see* A-70267
1α,2α-Epoxy-4β,5-dihydroyomogin, *in* Y-70001
3,4-Epoxy-2,2-dimethyl-1-butanol, *see* D-60431
8,16-Epoxy-8*H*,16*H*-dinaphtho[2,1-*b*:2′,1′-*f*][1,5]dioxocin, E-70014
5,6-Epoxy-7,9,11,14-eicosatetraenoic acid, E-60015
11,12-Epoxy-5,8,14-eicosatrienoic acid, E-60017
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▷ 1,2-Epoxy-4-(epoxyethyl)cyclohexane, *see* O-80056

1,10-Epoxy-11(13)-eremophilen-12-oic acid, E-80023
1,10-Epoxy-11(13)-eremophilen-12,8-olide, E-80024
1β,10β-Epoxy-11αH-eremophilen-12,8β-olide, *in* E-80024
10α,14-Epoxyestafiatin, *in* E-80057
10β,14-Epoxyestafiatin, *in* E-80057
▷ 1,2-Epoxy-1,1,2,2-ethanetetracarbonitrile, *see* T-80023
4β,15-Epoxy-1β-ethoxy-4Z-*millerenolide*, *in* M-60137
▷ 1-Epoxyethyl-3,4-epoxycyclohexane, *see* O-80056
▷ 3-(Epoxyethyl)-7-oxabicyclo[4.1.0]heptane, *see* O-80056
1α,2α-Epoxy-4,11(13)-eudesmadien-12,8β-olide, *in* Y-70001
6,15-Epoxy-1,4-eudesmanediol, E-80025
ent-5α,11-Epoxy-1β,4α,6α,8α,9β,14-eudesmanehexol, E-60018
1,4-Epoxy-6-eudesmanol, E-60019
1,4-Epoxy-6-eudesmanol, E-80026
8,12-Epoxy-3,7,11-eudesmatrien-1-ol, E-60020
3,4-Epoxy-11(13)-eudesmen-12-oic acid, E-60021
6,13-Epoxy-3-eunicellene-8,9,12-triol, E-80027
▷ 1,2-Epoxy-3-fluoropropane, *see* F-70032
22,25-Epoxy-2,3,6,26-furostanetetrol, E-70015
22S,25S-Epoxy-5-furostene-3β,26-diol, *see* N-60062
22,25-Epoxy-5-furostene-2α,3β,26-triol, *in* E-70015
Epoxyganoderiol *A*, *in* E-70013
Epoxyganoderiol *B*, *in* E-70025
Epoxyganoderiol *C*, *in* E-70025
1,10-Epoxy-4,11(13)-germacradien-12,8-olide, E-60022
4,5-Epoxy-1(10),7(11)-germacradien-8-one, E-60023
4α,5α-Epoxy-1(10)E-germacrene-6β,8β-diol, *see* S-70039
11,12-Epoxy-10(14)-guaien-4-ol, E-80028
3α,4α-Epoxy-10(14)-guaien-6α,12-olide, *in* E-80057
1β,10α-Epoxyhaageanolide, *in* H-60001
9,10-Epoxy-1-heptadecene-4,6-diyn-3-ol, *see* P-80006
3,4-Epoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]nonane, *in* H-80047
8,9-Epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-en-4-ol, *in* M-80202
1β,10β-Epoxy-8α-hydroxyachillin, *in* H-60100
ent-15,16-Epoxy-4α-hydroxy-13(16),14-clerodadiene-3,12-dione, E-80029
ent-15,16-Epoxy-2β-hydroxy-13(16),14-clerodadien-3-one, *in* E-80016
ent-3α,4α-Epoxy-2α-hydroxy-13-cleroden-15,16-olide, *in* E-80019
ent-3α,4α-Epoxy-16ξ-hydroxy-13-cleroden-15,16-olide, *in* E-80019
3,4-Epoxy-5-hydroxy-1-cyclohexenecarboxylic acid, E-80030
14,15-Epoxy-5-hydroxy-6,8,10,12-eicosatetraenoic acid, E-70016
14,15-Epoxy-20-hydroxy-5,8,11-eicosatrienoic acid, E-70018
5,6-Epoxy-20-hydroxy-8,11,14-eicosatrienoic acid, E-70017
1,10-Epoxy-13-hydroxy-7(11)-eremophilen-12,8-olide, E-80031
1β,10β-Epoxy-2α-hydroxy-11αH-eremophilen-12,8β-olide, *in* E-80024
1β,10β-Epoxy-2α-hydroxy-11βH-eremophilen-12,8β-olide, *in* E-80024
1β,10β-Epoxy-3α-hydroxy-11βH-eremophilen-12,8β-olide, *in* E-80024
1α,2α-Epoxy-10α-hydroxy-11(13)-eremophilen-12,8β-olide, *in* H-80159
1β,10β-Epoxy-2α-hydroxy-11(13)-eremophilen-12,8β-olide, *in* E-80024
1,2-Epoxy-3-hydroxy-4,11(13)-eudesmadien-12,8-olide, E-70019
4α,5α-Epoxy-3α-hydroxy-11(13)-eudesmen-12,8β-olide, *in* H-60136
4α,5α-Epoxy-3β-hydroxy-11(13)-eudesmen-12,8β-olide, *in* H-60136
4α,15-Epoxy-3α-hydroxyisoalantolactone, *in* I-80046
15,16-Epoxy-11β-hydroxy-8-isopimaren-7-one, *in* E-80033
8α,13R-Epoxy-6β-hydroxy-14-labden-11-one, *in* E-80037
24S,25S-Epoxy-26-hydroxy-7,9(11)-lanostadien-3-one, *in* E-70025
5,6-Epoxy-4-hydroxy-2-methoxy-2-cyclohexen-1-one, *see* H-70155
5,6-Epoxy-2-hydroxymethyl-2-cyclohexene-1,4-dione, *see* H-70181
12,16-Epoxy-18-hydroxy-20-nor-5(10),6,8,12,15-abietapentaene-11,14-dione, *see* I-60138
6,7-Epoxy-5-hydroxyocimene, *see* E-80042
ent-8α,14α-Epoxy-3β-hydroxy-9(11),15-pimaradiene-2,12-dione, E-80032
ent-8β,14β-Epoxy-3β-hydroxy-9(11),15-pimaradiene-2,12-dione, *in* E-80032
15,20-Epoxy-3β-hydroxy-14,15-seco-5,15,17(20)-pregnatriene-2,14-dione, *in* A-70267
24,25-Epoxy-23-hydroxy-7-tirucallen-3-one, *see* N-70036
6′,7′-Epoxy-5′α-hydroxytriptiliocoumarin, *in* T-80363
4α,15-Epoxyisoalantolactone, *in* I-80046
Epoxyisodihydrorhodophytin, E-60024
15,16-Epoxy-8-isopimaren-7-one, E-80033
2,3-Epoxy-6-isopropyl-3-methylcyclohexanone, *see* P-80153
Epoxyjaeschkeanadiol *p-hydroxybenzoate*, *in* J-70001
Epoxyjaeschkeanadiol vanillate, *in* J-70001
ent-11α,16α-Epoxy-17-kauranol, E-80034
1α,10β-Epoxykurubaschic acid benzoate, *in* K-60014
1β,10α-Epoxykurubashic acid angelate, *in* K-60014
1β,10α-Epoxykurubashic acid benzoate, *in* K-60014
9,13-Epoxy-7,14-labdadiene-2,3,20-triol, E-80035
14,15-Epoxy-8(17),12-labdadien-16-oic acid, E-60025
ent-8,13-Epoxy-14,15,19-labdanetriol, E-70020
8,13-Epoxy-3-labdanol, E-70021
ent-15,16-Epoxy-7,13(16),14-labdatriene, E-70022
15,16-Epoxy-8(17),13(16),14-labdatrien-19-oic acid, *see* L-60011
8,13-Epoxy-14-labdene, E-70023
ent-9,13-Epoxy-7-labdene-15,17-dioic acid, E-70024
8,20-Epoxy-14-labdene-2,3,7,13-tetrol, E-80036
8,13-Epoxy-14-labden-11-one, E-80037
2,9-Epoxylactarotropone, E-80038
24,25-Epoxy-7,9(11)-lanostadiene-3,26-diol, E-70025
21,23-Epoxylanosta-7,24-diene-3,21-diol, *see* F-70013
Epoxylaphodione, *in* D-60470
(Z)-6,7-Epoxyligustilide, *in* L-60026
20(29)-Epoxy-3-lupanol, E-60026
1,2-Epoxy-*p*-menthan-3-one, *see* P-80153
1,2-Epoxy-3-mercaptopropane, *see* M-80173
4β,15-Epoxy-1β-methoxy-9Z-*millerenolide*, *in* M-60137
2,3-Epoxy-2-methyl-1-butanol, *see* D-80462
2,3-Epoxy-3-methyl-1-butanol, *see* D-70426
3,4-Epoxy-2-methyl-1-butene, *see* M-70080
1,2-Epoxy-1-methylcyclohexane, *see* M-80125
2-(3,4-Epoxy-4-methylcyclohexyl)-6-methyl-2,5-heptadiene, *see* E-60009
1,2-Epoxy-1-methylcyclopentane, *see* M-80126
22S,25-Epoxy-24-methyl-3,11,20-furostanetriol, E-80039
8,19-Epoxy-17-methyl-1(15)-trinervitene-2,3,7,9,14,17-hexol, E-80040
4β,15-Epoxy-1(10)E,8E-millerdienolide, *in* M-60136
4α,13-Epoxymuzigadial, *in* M-80201
24,25-Epoxy-29-nor-3-cycloartanol, E-70026
1,3-Epoxy-2-nor-1,10-seco-1(5),3-aromadendradien-10-one, E-80041
2,3-Epoxy-5,7-octadien-4-ol, E-80042
13β,28-Epoxy-11-oleanene-3β,16β,23-triol, *see* S-60001
1α,2α-Epoxy-3-oxo-11(13)-eudesmen-12,8β-olide, *in* Y-70001
15,16-Epoxy-12-oxo-8(17),13(16),14-labdatrien-19-oic acid, *in* L-60011
(20S,22S)-21,24S-Epoxy-1-oxo-2,5,25-withatrienolide, *see* D-60003
1,2-Epoxy-1,1,3,3,3-pentafluoro-2-(trifluoromethyl)propane, *see* D-80158
5,6-Epoxy-4,16,20,22,23-pentahydroxy-1-oxo-ergost-2-en-26-oic acid γ-lactone, *see* W-60007
2,3-Epoxy-4-penten-1-ol, *see* V-80009
1,2-Epoxyperfluoroisobutene, *see* D-80158
11,15-Epoxy-3(20)-phytene-1,2-diol, E-80043
▷ 1,2-Epoxypropane, *see* M-70100
2,3-Epoxy-1-propanethiol, *see* M-80173
5-(1,2-Epoxypropyl)benzofuran, *see* M-70101
Epoxypteryxin, *in* K-70013
5,6-Epoxyquinoline, E-60027
7,8-Epoxyquinoline, E-60028
15,16-Epoxy-13,17-spatadiene-5,19-diol, E-60029
3,4-Epoxy-13(15),16-sphenolobadiene-5,18-diol, E-60030
3,4-Epoxy-13(15),16,18-sphenolobatrien-5-ol, E-60031
11,12-Epoxy-14-taraxeren-3-ol, E-80044
5,8-Epoxy-4,6,8-tetradecatriene-10,12-diyn-3-one, *see* H-80048
▷ Epoxytetrafluoroethane, *see* T-60049
2,3-Epoxy-1,1,1,3-tetrafluoropropane, *see* F-80070
9,10-Epoxy-7,8,9,10-tetrahydro-7,8-dihydroxybenzo[*a*]pyrene, *see* T-70041
8,13-Epoxy-1,6,7,9-tetrahydroxy-14-labden-11-one, E-70027
14,15-Epoxy-3,7,11,15-tetramethyl-2,6,10-hexadecatrienal, E-80045
21,23-Epoxy-7,24-tirucalladien-3-ol, E-60032
21,23-Epoxy-7,24-tirucalladien-3-one, *in* E-60032
12,13-Epoxytrichothec-9-en-3-ol, E-70028
3,4-Epoxy-1,5-tridecadiene-7,9,11-triyne, *see* P-80170
5,6-Epoxy-1,3-tridecadiene-7,9,11-triyne, *see* B-80277
1,2-Epoxy-3-tridecene-5,7,9,11-tetrayne, *in* T-80252
Epoxytrifluoroethane, *see* T-60305
2,3-Epoxy-1,1,1-trifluoropropane, *see* T-60294
2,3-Epoxy-1,4,8-trihydroxy-7(11)-eudesmen-12,8-olide, E-60033
ent-7β,20-Epoxy-1β,14α,20-trihydroxy-16-kauren-15-one, E-80046
8α,13R-Epoxy-6β,7β,9-trihydroxy-14-labden-11-one, *in* E-80037
5β,6β-Epoxy-4β,17α,20R-trihydroxy-3β-methoxy-1-oxo-8(14),24-withadienolide, *see* P-60144
6,7-Epoxy-5,20,22-trihydroxy-1-oxoergost-2-en-26-oic acid δ-lactone, *see* I-60143
5β,6β-Epoxy-4β,16β,20R-trihydroxy-1-oxo-22R,24R,25R-with-2-enolide, *see* W-60008
6α,7α-Epoxy-5α,14α,20R-trihydroxy-1-oxo-22R,24S,25R-with-2-enolide, *in* I-60143
2,3-Epoxy-4,5,8-trihydroxy-2-prenyl-1-tetralone, *see* D-70277
17*a*,21-Epoxy-4,4,8-trimethyl-D(17*a*)-homopregna-17,20-diene-12α,16β-diol 12-acetate, *see* F-70057
5,6-Epoxy-6,10,14-trimethyl-9,13-pentadecadien-2-one, E-80047

8,19-Epoxy-1(15)-trinervitene-2,3,7,9,14,17-hexol, E-80048
1α,2α-Epoxyyomogin, *in* Y-70001
▷ Equisetic acid, *see* A-70055
Eranthemoside, E-60034
9,11(13)-Eremophiladien-12-oic acid, E-70029
11-Eremophilene-2,8,9-triol, E-70030
1(10)-Eremophilen-7-ol, E-70031
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7,22-Ergostadiene-3,6-diol, *see* M-80058
5,24(28)-Ergostadiene-3,4,7,20-tetrol, *see* M-60070
7,22-Ergostadiene-3,5,6-triol, *see* M-70057
7,22-Ergostadien-3-ol, *see* M-80059
7,22-Ergostadien-3-one, *in* M-80059
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10(20),16-Ericacadien-19-oic acid, E-80050
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▷ Etenzamide, *in* H-70108
Ethanebis(dithioic)acid, E-60040
▷ Ethanedihydroxamic acid, *see* O-60048
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4,4′-(1,2-Ethanediyl)bis[1,2-benzenediol], *see* T-60101
5,5′-(1,2-Ethanediyl)bis[1,2,3-benzenetriol], *see* H-60062
5,5′-(1,2-Ethanediyl)bis-1,3-benzodioxole, *in* T-60101
6,6′-(1,2-Ethanediyl)bis-1,3-benzodioxol-4-ol, *in* H-60062
2,2′-(1,2-Ethanediyl)bisbenzoic acid, *see* B-80071
1,1′-(1,2-Ethanediyl)bishydrazine, *see* D-60192
2,2′-[1,2-Ethanediylbis(oxy)]bisethanamine, *see* B-60139
2,2′-[1,2-Ethanediylbis(thio)]bisethanethiol, *see* B-70150
2,2′-[1,2-Ethanediylbis(thio)]bisethanol, *see* B-70145
2,2′-(1,2-Ethanediylidene)bistricyclo[3.3.1.1^{3,7}]decane, *see* B-60075
1,1′,1″,1‴-1,2-Ethanediylidenetetrakiscyclopropane, *see* T-60034
S_6-Ethano-18, *see* H-70087
1,10-Ethanodibenzo[*a,e*]cyclooctene, *see* C-60229
13,15-Ethano-3,17-diethyl-2,12,18-trimethylmonobenzo[*g*]porphyrin, E-60042
13,15-Ethano-17-ethyl-2,3,12,18-tetramethylmonobenzo[*g*]porphyrin, E-60043
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2,2′-(1,2-Ethenediyl)bisbenzofuran, *see* D-80069
2,2′-(1,2-Ethenediyl)bisfuran, *see* D-60191
2,2′-(1,2-Ethenediyl)bis-1*H*-indole, *see* D-80395
15,15′-(1,2-Ethenediyl)bis[2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin], *see* B-60142
2,2′(1,2-Ethenediyl)bisphenol, *see* D-80378
3,3′-(1,2-Ethenediyl)bisphenol, *see* D-80381
4,4′-(1,2-Ethenediyl)bisphenol, *see* D-80385
1,1′-(1,2-Ethenediylidene)biscyclohexane, *see* B-80144
2,2′,2″,2‴-(1,2-Ethenediylidene)tetrakis[9,10-dihydro-1′,2′-benzenoanthracene], *see* T-60169
1,1′,1″,1‴-[1,2-Ethenediylidenetetrakis(oxy)]tetrakisbenzene, *see* T-80157
▷ Ethenetetracarbonitrile, *see* T-60031
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2,6-(Etheno[1,4]benzenoetheno)naphthalene, *see* N-70006
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N^2,3-Ethenoguanosine, *in* I-70006
12,15-Etheno-5,9-metheno-9*H*-benzocyclotridecene, *see* B-70036
5,8-Etheno-17,13-metheno-13*H*-dibenzo[*a,g*]cyclotridecene, *see* D-70071
1,14-Ethenonaphtho[1′,8′:5,6,7]cyclohepta[1,2,3,4-*def*]phenanthrene, *see* H-80037
α-Ethenylbenzeneacetic acid, *see* P-80096
4-Ethenyl-1,3-benzenediol, *see* V-70010
5-Ethenyl-4,6-benzofurandiol, *see* D-70352
5-Ethenyl-6-benzofuranol, *see* H-70231
▷ 5-Ethenylbicyclo[2.2.1]hept-2-ene, E-70036
N-Ethenylcarbazole, *see* V-80007
3-Ethenylcyclohexene, *see* V-60009
5-Ethenyl-1-cyclopentenecarboxylic acid, *see* V-60010
3-Ethenyl-2-cyclopenten-1-ol, *see* V-80008
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2-Ethenyl-1,1-cyclopropanedicarboxylic acid, *see* V-60011
3-Ethenylcyclopropene, *see* V-60012
3-Ethenyldihydro-2(3*H*)-furanone, *see* D-70279
1-Ethenyl-2,4-dimethoxybenzene, *in* V-70010
5-Ethenyl-4,6-dimethoxybenzofuran, *in* D-70352
5-Ethenyl-1,6-dimethyl-2,7-phenanthrenediol, *see* D-70294
7-Ethenyldodecahydro-1,1,4*a*,7-tetramethyl-8*a*(2*H*)-phenanthrenol, *see* H-60163
6-Ethenyl-11-ethyl-15,19,20,21-tetrahydro-18-hydroxy-5,10,22,23-tetramethyl-4,7-imino-2,21-methano-14,16-metheno-9,12-nitrilo-17*H*-azuleno[1,8-*bc*][1,5]diazacyclooctadecin-17-one, *see* C-60230
4-Ethenylhexahydro-4,7*a*-dimethyl-2(3*H*)-benzofuranone, *see* A-70206
2-Ethenyl-4-hydroxybenzenepropanoic acid, *see* H-70232
4,4′-Ethenylidenebismorpholine, *see* D-70447
1,1′-Ethenylidenebispiperidine, *see* D-70500
4-Ethenyl-1*H*-imidazole, *see* V-70012
2-Ethenyl-1*H*-indole, *see* V-70013
1-Ethenyl-4-methoxybenzene, *in* H-70209
5-Ethenyl-5-methyl-1,3-cyclopentadiene, *see* M-70146
1-Ethenyl-3-methylcyclopentene, *see* M-80189
2-Ethenyl-3-(1-nonen-3,5,7-triynyl)oxirane, *see* P-80170
3-Ethenyl-2-oxiranemethanol, *see* V-80009
▷ 4-Ethenylphenol, *see* H-70209
5-Ethenyl-5′-(1-propenyl)-2,2′-bithienyl, *see* P-80182
5-Ethenyl-2-pyrimidinamine, *see* A-60269
2-Ethenyl-1*H*-pyrrole, *see* V-60013
4-Ethenylquinoline, *see* V-70014
[(Ethenylsulfonyl)methyl]benzene, *in* B-80062
2-(5-Ethenyltetrahydro-5-methyl-2-furanyl)-4,4-dimethyl-5-hexen-3-one, *see* A-60305
4-Ethenyl-1,2,3-thiadiazole, *see* V-60014
5-Ethenyl-1,2,3-thiadiazole, *see* V-60015
[(Ethenylthio)methyl]benzene, *see* B-80062
3-Ethenylthiophene, *see* V-80010
5-Ethenyluridine, *see* V-70015
▷ Ethenzamide, *in* H-70108
1-Ethoxy-9*Z*-*millerenolide*, *in* M-60137
α-Ethoxyacrylic acid, *see* E-70037
β-Ethoxyacrylonitrile, *see* E-80059
▷ 2-Ethoxybenzamide, *in* H-70108
4-Ethoxy-3(2*H*)-benzofuranone, *in* H-80108
2-Ethoxybenzoic acid, *in* H-70108
1-Ethoxy-9*H*-carbazole, *in* H-80137
2-Ethoxycarbazole, *in* H-60109
2-Ethoxycarbonylcyclopentanone, *in* O-70084
Ethoxycarbonylmalonaldehyde, *in* D-60190
5-Ethoxy-3,4-dihydro-2*H*-pyrrole, *in* P-70188
7-Ethoxy-3,4-dimethylcoumarin, *in* H-60119
5-Ethoxy-2,4-dinitrophenol, *in* D-80491
▷ (1-Ethoxyethyl) hydroperoxide, *see* E-60044
4-Ethoxy-2(5*H*)-furanone, *in* F-80087
N-Ethoxy-1,1,1,1′,1′,1′-hexafluorodimethylamine, *in* B-60180
▷ 1-Ethoxy-1-hydroperoxyethane, E-60044
10α-Ethoxy-3β-hydroxy-4,11(13)-cadinadien-12-oic acid, *in* Z-70001
2-Ethoxy-3-hydroxyquinoxaline, *in* D-60279
4-Ethoxy-2-hydroxy-*N,N,N*-trimethyl-4-oxo-1-butanaminium, *in* C-70024
3-Ethoxy-1*H*-isoindole, *in* P-70100
6-Ethoxy-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran, *in* D-70365
9-(Ethoxymethyl)-4-formyl-3,8-dihydroxy-1,6-dimethyl-11-oxo-11*H*-dibenzo[*b,e*][1,4]dioxepin-7-carboxylic acid, *see* C-70035
▷ 2-Ethoxymethyl-3-hydroxy-1-methoxyanthraquinone, *in* D-70306
4-Ethoxy-1,2-naphthoquinone, *in* H-60194
4-Ethoxy-2-nitropyridine, *in* N-70063
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2-Ethoxy-1-pyrroline, *in* P-70188
3-Ethoxy-2-quinoxalinol, *in* D-60279
3-Ethoxy-2(1*H*)quinoxalinone, *in* D-60279
α-Ethoxystyrene, *in* P-60092
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▷ Ethyl acrylate, *in* P-70121
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3-(2-Ethyl-2-butenyl)-9,10-dihydro-1,6,8-trihydroxy-9,10-dioxo-2-anthracenecarboxylic acid, E-70038
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3-Ethyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one, E-70040
3-Ethyl-5,7-dihydroxychromone, *see* E-70040
6-Ethyl-2,4-dihydroxy-3-methylbenzoic acid, E-70041
3-Ethyl-2,19-dioxabicyclo[16.3.1]docosa-3,6,9,18(22),21-pentaen-12-yn-20-one, E-70042
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2-Fluoro-3-hydroxybenzaldehyde, F-60035
2-Fluoro-5-hydroxybenzaldehyde, F-60036
4-Fluoro-3-hydroxybenzaldehyde, F-60037
2-Fluoro-5-hydroxybenzoic acid, F-60038
2-Fluoro-6-hydroxybenzoic acid, F-60039
3-Fluoro-2-hydroxybenzoic acid, F-60040
3-Fluoro-4-hydroxybenzoic acid, F-60041
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4-Fluoro-3-hydroxybenzoic acid, F-60043
5-Fluoro-2-hydroxybenzoic acid, F-60044
2-Fluoro-3-hydroxytoluene, *see* F-60052
2-Fluoro-4-hydroxytoluene, *see* F-60057
2-Fluoro-5-hydroxytoluene, *see* F-60059
2-Fluoro-6-hydroxytoluene, *see* F-60056
3-Fluoro-2-hydroxytoluene, *see* F-60055
3-Fluoro-4-hydroxytoluene, *see* F-60053
4-Fluoro-2-hydroxytoluene, *see* F-60060
4-Fluoro-3-hydroxytoluene, *see* F-60054
5-Fluoro-2-hydroxytoluene, *see* F-60058
3-Fluoro-1*H*-indole, F-80043
4-Fluoro-1*H*-indole, F-80044
5-Fluoro-1*H*-indole, F-80045
6-Fluoro-1*H*-indole, F-80046
7-Fluoro-1*H*-indole, F-80047
2-Fluoro-6-iodobenzoic acid, F-70020
3-Fluoro-2-iodobenzoic acid, F-70021
3-Fluoro-4-iodobenzoic acid, F-70022
4-Fluoro-2-iodobenzoic acid, F-70023
4-Fluoro-3-iodobenzoic acid, F-70024
5-Fluoro-2-iodobenzoic acid, F-70025
1-Fluoro-3-iodopropane, F-70026
2-Fluoro-3-iodopyridine, F-80048
2-Fluoro-4-iodopyridine, F-60045
3-Fluoro-4-iodopyridine, F-60046
4-Fluoro-1(3*H*)-isobenzofuranone, F-70027
7-Fluoro-1(3*H*)-isobenzofuranone, F-70028
▷ 1-Fluoro-2-isocyanatobenzene, F-60047
▷ 1-Fluoro-3-isocyanatobenzene, F-60048
▷ 1-Fluoro-4-isocyanatobenzene, F-60049
1-Fluoro-4-isothiocyanatobenzene, F-80049
2-Fluorolepidine, *see* F-80050
3-Fluorolepidine, *see* F-80051
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Fluoromaleic anhydride, *in* F-80030
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2-Fluoro-6-mercaptoaniline, *see* A-80073
3-Fluoro-2-mercaptoaniline, *see* A-80075
3-Fluoro-4-mercaptoaniline, *see* A-80076
4-Fluoro-2-mercaptoaniline, *see* A-80074
1-Fluoro-2-mercaptobenzene, *see* F-80018
1-Fluoro-3-mercaptobenzene, *see* F-80019
1-Fluoro-4-mercaptobenzene, *see* F-80020
2-Fluoro-4-mercaptobenzoic acid, F-70029
2-Fluoro-6-mercaptobenzoic acid, F-70030
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2-Fluoro-5-methoxybenzoic acid, *in* F-60038
3-Fluoro-4-methoxybenzoic acid, *in* F-60041
5-Fluoro-2-methoxybenzoic acid, *in* F-60044
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1-Fluoro-2-methoxy-4-methylbenzene, *in* F-60054

1-Fluoro-3-methoxy-6-methylbenzene, *in* F-60057
1-Fluoro-4-methoxy-3-methylbenzene, *in* F-60059
2-Fluoro-1-methoxy-4-methylbenzene, *in* F-60053
4-Fluoro-2-methoxy-1-nitrobenzene, *in* F-60061
2-Fluoro-4-methoxytoluene, *in* F-60057
2-Fluoro-5-methoxytoluene, *in* F-60059
3-Fluoro-4-methoxytoluene, *in* F-60053
4-Fluoro-3-methoxytoluene, *in* F-60054
2-Fluoro-4-methylanisole, *in* F-60053
2-Fluoro-5-methylanisole, *in* F-60054
3-Fluoro-4-methylanisole, *in* F-60057
4-Fluoro-3-methylanisole, *in* F-60059
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2-Fluoro-4-methylphenol, F-60053
2-Fluoro-5-methylphenol, F-60054
2-Fluoro-6-methylphenol, F-60055
3-Fluoro-2-methylphenol, F-60056
3-Fluoro-4-methylphenol, F-60057
4-Fluoro-2-methylphenol, F-60058
4-Fluoro-3-methylphenol, F-60059
5-Fluoro-2-methylphenol, F-60060
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3-Fluoro-4-methylquinoline, F-80051
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6-Fluoro-2-methylquinoline, F-80053
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2-Fluoro-6-(methylthio)benzonitrile, *in* F-70030
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▷ 5-Fluoro-2-nitrophenol, F-60061
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18-Fluoro-9-octadecenoic acid, F-80057
1-Fluorooctane, F-80058
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ω-Fluorooleic acid, *see* F-80057
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α-Fluoro-α-phenylbenzeneacetaldehyde, *see* F-60033
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▷ Formoononetin, *see* H-80190
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Helicascolide A, H-80004
Helicascolide B, *in* H-80004
Helichromanochalcone, H-80005
Helichrysin, *in* H-80246
Helicquinone, H-60015
Heliettin, *see* C-60031
Helihumulone, H-80006
Helikrausichalcone, H-80007
Helilupulone, H-80008
Heliopsolide, H-70007
Helipterol, H-80009
Helisplendidilactone, H-80010
Helminthosporal, H-60016
Helogynic acid, H-70008
▷ Helvolic acid, H-80011
Helvolinic acid, *in* H-80011
Hemerocallin, *see* S-50130
Hemicyclone, *see* D-70403
sym-Hemimellitenol, *see* T-60371
m-Hemipic acid, *in* D-60307
Heneicosanedioic acid, H-80012
Heneicosanoic acid, H-80013
26-Henpentacontanone, H-70009
Henricine, H-60017
12,14-Hentriacontanedione, H-80014
14,16-Hentriacontanedione, H-80015
Hentriacontanoic acid, H-80016
1,14,34,35,36,37,38-Heptaazaheptacyclo[12.12.7.1^{3,7}.1^{8,12}.1^{16,20}.1^{21,25}.1^{28,32}]octatriaconta-3,5,7(38),8,10,12(37),16,18,20(36),21,23,25(35),28,30,32(34)pentadecane, H-70010
7,16-Heptacenedione, H-60018
7,16-Heptacenequinone, *see* H-60018
13-Heptacosene, H-60019
Heptacyclo[7.7.0.0^{2,6}.0^{3,15}.0^{4,12}.0^{5,10}.0^{11,16}]hexadeca-7,13-diene, H-70011
Heptacyclo[7.7.0.0^{2,6}.0^{3,15}.0^{4,12}.0^{5,10}.0^{11,16}]hexadecane, *in* H-70011
Heptacyclo[19.3.0.0^{1,5}.0^{5,9}.0^{9,13}.0^{13,17}.0^{17,21}]tetracosane, H-80017
Heptacyclo[6.6.0.0^{2,6}.0^{3,13}.0^{4,11}.0^{5,9}.0^{10,14}]tetradecane, H-70012
Heptacyclo[9.3.0.0^{2,5}.0^{3,13}.0^{4,8}.0^{6,10}.0^{9,12}]tetradecane, H-70013
Heptacyclo[5.5.1.1^{4,10}.0^{2,6}.0^{3,11}.0^{5,9}.0^{8,12}]tetradecane, *see* H-70012
4,6-Heptadecadiyne-3,8,9-triol, *in* D-80321
8,10,12,14-Heptadecatetraen-1-al, H-80018
1,7,9,15-Heptadecatetraene-11,13-diyne, H-80019
1,9,15-Heptadecatriene-11,13-diyn-8-ol, H-80020
1,9,16-Heptadecatriene-4,6-diyn-3-ol, H-80021
2,9,16-Heptadecatriene-4,6-diyn-1-ol, H-80022
2,9,16-Heptadecatriene-4,6-diyn-8-ol, H-80023
1-Heptadecene-4,6-diyne-3,9,10-triol, H-80024
2,4-Heptadienal, H-60020
2,4-Heptadienoic acid, H-60021

2,4-Heptadien-1-ol, H-70014
1,5-Heptadien-3-one, H-70015
1,5-Heptadien-4-one, H-70016
1,6-Heptadien-3-one, H-70017
4,5-Heptadien-3-one, H-70018
1,5-Heptadiyne, H-80025
▷ Heptafluorobromopropane, *see* B-80206
1,1,2,2,3,3,3-Heptafluoro-1-iodopropane, H-80026
1,2,3,4,5,6,7-Heptafluoronaphthalene, H-70019
1,2,3,4,5,6,8-Heptafluoronaphthalene, H-70020
1*H*-Heptafluoronaphthalene, *see* H-70019
2*H*-Heptafluoronaphthalene, *see* H-70020
▷ Heptafluoropropyl bromide, *see* B-80206
3,4-Heptafulvalenedione, H-60022
8-(8-Heptafulvenyl)-*p*-tropoquinone methide, *see* C-70222
3″,4′,4‴,5,5″,7,7″-Heptahydroxy-3,8″-biflavanone, *see* G-70005
2,3,5,14,20,22,25-Heptahydroxy-7-cholesten-6-one, H-60023
1,2,4,6,8,9,14-Heptahydroxydihydro-β-agarofuran, H-80027
3′,4′,4″,5,5″,7,7″-Heptahydroxy[3,8]flavanonylflavone, *see* D-80209
3,3′,4′,5,5′,7,8-Heptahydroxyflavone, H-70021
3,3′,4′,5,6,7,8-Heptahydroxyflavone, H-80028
3′,4′,5,5′,6,7,8-Heptahydroxyflavone, H-80029
3′,4′,5,5′,6,7,8-Heptamethoxyflavanone, *in* H-80029
3,3′,4′,5,5′,7,8-Heptamethoxyflavone, *in* H-70021
3,4-Heptamethylenefuran, *see* H-60047
▷ Heptamethyleneimine, *see* O-70010
4,6,8,10,12,14,16-Heptamethyl-6,8,11-octadecatriene-3,5,13-trione, H-70022
1,5-Heptanediol, H-80030
1,7-Heptanedithiol, H-70023
5-Heptenenitrile, *in* H-70024
5-Heptenoic acid, H-70024
6-(1-Heptenyl)-5,6-dihydro-2*H*-pyran-2-one, H-60025
8-(3-Heptyloxiranyl)-1-octene-4,6-diyn-3-ol, *see* P-80006
2-Heptyl-12-oxo-13-henicosenoic acid, *see* F-60012
2-Heptyl-10-oxo-11-nonadecenoic acid, *see* F-60011
6-Heptyne-2,5-diamine, H-60026
4-Heptynenitrile, *in* H-80032
6-Heptynenitrile, *in* H-80033
3-Heptynoic acid, H-80031
4-Heptynoic acid, H-80032
6-Heptynoic acid, H-80033
6-Heptyn-2-one, H-70025
Herbacin, H-60027
Herbicidal substance 1328-3, *in* M-70134
Herbicidal substance 1328-2, *see* M-70134
Hercycin, *see* H-60083
Heritol, H-60028
Heritonin, H-80034
Hermosillol, H-60029
Herpetetrone, H-70026
Herzynine, *see* H-60083
Hesperidene, *see* I-70087
heta, *see* T-60016
11-HETE, *see* H-60130
12-HETE, *see* H-60131
5-HETE, *see* H-60127
8-HETE, *see* H-60128
9-HETE, *see* H-60129
▷ Heteroauxin, *see* I-70013
Heterobryoflavone, H-70027
Heterocoerdianthrone, *see* D-70073
Heteronemin, H-60030
2α,5α,7β,9α,10β,13α-Hexaacetoxy-4β,20-epoxy-11-taxene, *see* B-80002
1β,2α,7β,9α,10β,13α-Hexaacetoxy-4β,20-epoxy-11-taxen-5α-ol, *in* B-80002
2α,4α,7β,9α,10β,13α-Hexaacetoxy-5β,20-epoxy-11-taxen-1β-ol, *see* B-80003
▷ Hexaaminobenzene, *see* B-80014
2*a*,4*a*,6*a*,8*a*,10*a*,12*a*-Hexaazacoronene-1,3,5,7,9,11(2*H*,4*H*,6*H*,8*H*,10*H*,12*H*)-hexone, H-80035
1,4,7,12,15,18-Hexaazacyclodocosane, H-70028
1,4,7,13,16,19-Hexaazacyclotetracosane, H-70029
1,5,6,10,10*a*,10*c*-Hexaazadibenzo[*a*,*f*]pentalene, *see* P-70169
3,9,17,23,29,30-Hexaaza-6,20-dioxatricyclo[23.3.1.1^{11,15}]triaconta-1(28),11(29),12,14,25,27-hexaene, H-80036
1,14,29,30,31,32-Hexaazahexacyclo[12.7.7.1^{3,7}.1^{8,12}.1^{16,20}.1^{23,27}]dotriaconta-3,5,7(32),8,10,12(31),16,18,20(30),23,25,27(29)-dodecaene, H-70030
1,4,5,8,9,12-Hexaazatriphenylenehexacarboxylic acid, *see* B-60051
Hexabenzohexacyclo[5.5.2.2^{4,10}.1^{1,7}.0^{4,17}.0^{10,17}]heptadecane, *see* C-70031
Hexabenzo[*bc*,*ef*,*hi*,*kl*,*no*,*qr*]coronene, H-60031
1,2,3,4,5,6-Hexa-*O*-benzoyl-*myo*-inositol, *in* I-80015
α,α′,3,4,5,6-Hexabromo-*o*-xylene, *see* T-80012
Hexabutylbenzene, H-60032
6,15-Hexacenedione, H-60033
▷ 2,2′,4,4′,5,5′-Hexachlorobiphenyl, H-60034
Hexa[7]circulene, H-80037
Hexacosanal, H-80038
Hexacyclo[4.4.0.0^{2,5}.0^{3,9}.O^{4,8}.0^{7,10}]decane, H-70032
Hexacyclo[11.3.1.1^{3,7}.1^{5,9}.1^{11,15}.0^{2,10}]eicos-2-ene, H-70031
Hexacyclo[26.2.2.2^{4,7}.2^{10,13}.2^{16,19}.2^{22,25}]tetraconta-4,6,10,12,16,18,22,24,28,30,31,33,35,37,39-pentadecaene, *see* P-80010
Hexacyclo[6.5.1.0^{2,7}.0^{3,11}.0^{4,9}.0^{10,14}]tetradeca-5,12-diene, H-80039
Hexacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}.0^{8,11}]undecan-4-one, H-60035
11,13-Hexadecadienal, H-70033
Hexadecahydro-10*a*,1,4-ethanylylidene-7,5,9,11-[1,2]propanediyl[3]ylidene-10*a*H-benzo[b]fluorene, *see* N-80067
8,9-Hexadecanedione, H-70034
15-Hexadecanolide, *in* H-80173
N-Hexadecanoylhomoserine lactone, *in* A-60138
7,9,11,13-Hexadecatetraen-1-al, H-80040
6,8,12,14-Hexadecatetraen-10-yn-1-ol, H-80041
6,8,14-Hexadecatriene-10,12-diyn-1-al, H-80042
1,6,8-Hexadecatriene-10,12,14-triyne, H-80043
7,12,14-Hexadecatrien-10-yn-1-ol, H-80044
2-Hexadecenal, H-60036
7-Hexadecenal, H-70035
5-Hexadecenoic acid, H-80045
5-Hexadecyne, H-60037
1,2,9,10,17,18-Hexadehydro[2.2.2]paracyclophane, H-60038
▷ 1,5-Hexadiene-3,4-diol, H-70036
1,5-Hexadiene-3,4-dione, H-60039
3,4-Hexadienoic acid, H-70037
3,5-Hexadienoic acid, H-70038
3,5-Hexadien-1-ol, H-70039
1,2-Hexadien-5-yne, H-70040
1,3-Hexadien-5-yne, H-70041
1,5-Hexadiyn-3-one, H-60040
3,5-Hexadiyn-2-one, H-60041
▷ 2,4-Hexadinophenone, *see* P-60109
3-[5-(2,4-Hexadiynyl)-2-furanyl]-2-propenal, H-80046
3-[2-(2,4-Hexadiynyl)-5-furyl]acrolein, *see* H-80046
2-(2,4-Hexadiynylidene)-1,6-dioxaspira[4.5]dec-3-en-8-ol, H-70042
2-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene, *in* H-70042
7-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.4]nona-2,8-dien-4-ol, *see* M-60154
7-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.4]nona-2,8-dien-4-ol, *see* M-80202
7-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.4]non-8-en-3-ol, H-80047
2-(2,4-Hexadiynylidene)-3,4-epoxy-1,6-dioxaspiro[4.5]decane, *in* H-70042
2-(2,4-Hexadiynylidene)-5-(propionylmethylidene)-2,5-dihydrofuran, H-80048
▷ Hexaethylbenzene, H-70043
Hexafluorobiacetyl, *see* H-60043
1,1,1,4,4,4-Hexafluoro-2,3-butanedione, H-60043
1,2,3,4,5,5-Hexafluoro-1,3-cyclopentadiene, H-60044
Hexafluoro(hexafluorocyclobutylidene)cyclobutane, *see* D-60513
Hexafluoroisobutylidene sulfate, *see* T-60311
1,1,1,1′,1′,1′-Hexafluoro-*N*-methoxydimethylamine, *in* B-60180
▷ Hexafluoro(methylenecyclopropane), *see* D-60185
1,2,3,4,5,6-Hexafluoronaphthalene, H-70044
1,2,4,5,6,8-Hexafluoronaphthalene, H-70045
1,1,1,2,2,3-Hexafluoropropane, H-80049
1,1,1,3,3,3-Hexafluoropropane, H-80050
α,α,α,α′,α′,α′-Hexafluoro-*m*-xylene, *see* B-60176
α,α,α,α′,α′,α′-Hexafluoro-*o*-xylene, *see* B-60175
α,α,α,α′,α′,α′-Hexafluoro-*p*-xylene, *see* B-60177
2,3,4,6,7,8-Hexahydro-1,5-anthracenedione, H-80051
Hexahydroazirino[2,3,1-*hi*]indol-2(1*H*)-one, H-70046
Hexahydro-4(1*H*)-azocinone, H-70047
Hexahydro-5(2*H*)-azocinone, H-70048
1,2,3,5,10,10*a*-Hexahydrobenz[*f*]indolizine, *see* H-70072
Hexahydro-2(3*H*)-benzofuranone, H-70049
1,2,3,4,7,8-Hexahydrobenzo[*c*]phenanthrene, H-80052
▷ Hexahydrobenzophenone, *see* B-70071
Hexahydro-1*H*-2-benzopyran-1,3(4*H*)-dione, *in* C-80023
2,3,4,4*a*,5,6-Hexahydro-7*H*-1-benzopyran-7-one, H-60045
1,3,4,6,7,11*b*-Hexahydro-2*H*-benzo[*a*]quinolizine, H-80053
2,3,6,7,10,11-Hexahydrobenzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]dithiin, H-70050
2,3,6,7,10,11-Hexahydrobenzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]oxathiin, H-70051
3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]oxazine, H-80054
3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]thiazine, H-80055
Hexahydro-2(3*H*)-benzoxazolone, H-70052
Hexahydro-2,5-bis(trichloromethyl)furo[3,2-*b*]furan-3*a*,6*a*-diol, H-70053
Hexahydrochroman-7-one, *see* O-60011
5,6,7,8,9,10-Hexahydro-4*H*-cyclonona[*c*]furan, H-60047
Hexahydro-1*H*-cyclopenta[*c*]furan-1-one, H-70054
Hexahydrocyclopenta[*cd*]pentalene-1,3,5(2*H*)-trione, H-60048
Hexahydro-2*H*-cyclopenta[*b*]thiophene, H-60049
1,2,3,4,4*a*,10*a*-Hexahydrodibenzo[*b*,*e*][1,4]dioxin, H-80056
1,5,6,8,12,13-Hexahydro-4,14:7,11-diethenodicyclopenta[*a*,*g*]cyclododecene, *see* I-60021
1,2,3,4,6,7-Hexahydro-6,7-dihydroxy-1,4-bis(phenylmethyl)-1,4-diazocine-5,8-dione, *see* D-80078

Hexahydro-3,7*a*-dihydroxy-3*a*,7-dimethyl-1,4-isobenzofurandione, H-70055
2,3,4,6,7,8-Hexahydro-4,8-dihydroxy-2-(1-hydroxyheptyl)-5*H*-1-benzopyran-5-one, H-80057
▷ 3,4,5,6,9,10-Hexahydro-14,16-dihydroxy-3-methyl-1*H*-2-benzoxacyclotetradecin-1,7(8*H*)-dione, *see* Z-60002
2,3,5,6,8,9-Hexahydro-1*H*-diimidazo[1,2-*d*:2′,1′-*g*][1,4]diazepine, H-80058
2-[(2,3,3*a*,4,5,7*a*-Hexahydro-3,6-dimethyl-2-benzofuranyl)ethylidene]-6-methyl-5-heptenoic acid, H-60050
2-[(3,4,4*a*,5,6,8*a*-Hexahydro-4,7-dimethyl-2*H*-1-benzopyran-2-yl)ethylidene]-6-methyl-5-heptenoic acid, H-60046
2,3,4,4*a*,5,6-Hexahydro-2,2-dimethyl-1,3-methanonaphthalen-7(1*H*)-one, *see* T-80242
1,2,3,4,5,6-Hexahydro-1,4-dimethyl-7-(1-methylethyl)azulene, *see* G-70031
1,2,5,7,8,8*a*-Hexahydro-4,8*a*-dimethyl-6-(1-methylethyl)-1-naphthalenol, *see* E-60064
4,4*a*,5,6,7,8-Hexahydro-2,5-dimethyl-5-(4-methyl-3-pentenyl)-1,8*a*(3*H*)-naphthalenedicarboxaldehyde, *see* P-60064
2*a*,3*a*,5*a*,6*a*,6*b*,6*c*-Hexahydro-3,6-dioxacyclopenta[*cd*,*gh*]pentalene, *see* D-70463
Hexahydro-2,6-dioxoimidazolo[4,5-*d*]imidazole, *see* T-70066
Hexahydro-1,4-dithiino[2,3-*b*]-1,4-dithiin, H-60051
Hexahydro-1,2,3,5-ethanediylidene-1*H*-cyclobuta[*cd*]pentalen-4(1*aH*)one, *see* H-60035
Hexahydro-2,6,3,5-ethanediylidene-2*H*,3*H*-1,4-dioxacyclopenta[*cd*]pentalene, *see* D-70461
Hexahydro-1,2,4-ethanylylidene-1*H*-cyclobuta[*cd*]pentalene-5,7(1*aH*)dione, *see* P-70022
Hexahydro-1,2,4-ethanylylidene-1*H*-cyclobuta[*cd*]pentalene-3,5,7-trione, *see* P-70023
1,2,3,6,7,8-Hexahydro-3*a*,5*a*-ethenopyrene, H-70056
Hexahydrofarnesol, *see* T-70282
Hexahydro-2*H*-furo[3,2-*b*]pyrrol-2-one, H-80059
Hexahydrohomophthalic acid, *see* C-80023
2,4,5,6,7,7*a*-Hexahydro-7*a*-hydroxy-3,6-dimethyl-2-benzofuranone, *see* P-80063
3*a*,4,5,8,9,11*a*-Hexahydro-9-hydroxy-6,10-dimethyl-3-methylenecyclodeca[*b*]furan-2(3*H*)-one, *see* H-60006
5-[Hexahydro-5-hydroxy-4-(3-hydroxy-4-methyl-1-octen-6-ynyl)-2(1*H*)-pentalenylidene]pentanoic acid, *see* I-60003
2,3,4,7,8,8*a*-Hexahydro-8-(5-hydroxy-4-methylpentyl)-6,8-dimethyl-1*H*-3*a*,7-methanoazulene-3-carboxylic acid, H-70057
Hexahydro-7-hydroxy-3-(2-methylpropyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, *see* C-60213
3,3*a*,4,5,8*a*,8*b*-Hexahydro-4-hydroxy-3,6,9-trimethylazuleno[4,5-*b*]furan-2,7-dione, *see* H-60100
1,2,3,6,7,8-Hexahydro-*as*-indacene, *see* H-60094
1,2,3,5,6,7-Hexahydro-*s*-indacene, *see* H-60095
3*a*,4,5,6,7,7*a*-Hexahydro-1*H*-inden-1-one, H-70058
2,3,5,6,7,8-Hexahydro-1*H*-indolizinium(1+), H-70059
1,3,3*a*,4,5,7*a*-Hexahydro-2*H*-indol-2-one, H-70060
Hexahydro-1(3*H*)-isobenzofuranone, H-70061
1,2,3,4,5,6-Hexahydro-7-isopropyl-1,4-dimethylazulene, *see* G-70031
1,2,6,7,8,8*a*-Hexahydro-6-isopropyl-4,8*a*-dimethyl-1-naphthol, *see* E-60064
Hexahydro-1,3(2*H*,4*H*)-isoquinolinedione, H-80060
Hexahydromandelic acid, *see* C-60212
2,3,3*a*,4,5,7*a*-Hexahydro-2,5-methano-1*H*-indene, *see* T-80236
2,3,4,5,6,7-Hexahydro-4,7-methano-1*H*-indene, *see* T-60260
3*a*,4,6*a*,7,9*a*,9*b*-Hexahydro-1,4,7-methano-1*H*-phenalene, *see* P-70021
4*b*,9*b*,10,14*b*,14*c*,15-Hexahydro-5,10,15-metheno-5*H*-benzo[*a*]naphth[1,2,3-*de*]anthracene, *see* T-70210
Hexahydro-1,3,5-methenocyclopenta[*cd*]pentalene-2,4,6(1*H*)-trione, *see* P-60031
Hexahydro-7-methylcyclopenta[*c*]pyran-1(3*H*)-one, *see* M-70150
3*a*,4,5,6,7,7*a*-Hexahydro-3-methylene-2-(3*H*)-benzofuranone, H-70062
Hexahydro-3-(1-methylpropyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, H-60052
Hexahydro-3-(2-methylpropyl)pyrrolo[1,2*a*]pyrazine-1,4-dione, *see* C-80185
Hexahydro-3-methylpyrrolo[1,2-*a*]pyrazine-1,4-dione, *see* C-80194
1,2,3,5,8,8*a*-Hexahydronaphthalene, H-60053
1,2,3,7,8,8*a*-Hexahydronaphthalene, H-60054
1,3,4,5,7,8-Hexahydro-2,6-naphthalenedione, H-70063
3,4,4*a*,5,8,8*a*-Hexahydro-1(2*H*)-naphthalenone, H-80061
4*a*,5,6,7,8,8*a*-Hexahydro-2(1*H*)-naphthalenone, H-80062
3,4,5,6,7,8-Hexahydronaphthalen-1(2*H*)-one-2-carboxylic acid, *see* O-80015
Hexahydronezukone, *see* I-70091
Hexahydronicotinic acid, *see* P-70102
1,2,6*b*,7,8,12*b*-Hexahydro-4,7,8,10,12*b*-pentahydroxy-3,9-perylenedione, *see* A-80052
1,2,3,4,5,6-Hexahydropentalene, H-70066
1,2,3,3*a*,4,5-Hexahydropentalene, H-70064
1,2,3,3*a*,4,6*a*-Hexahydropentalene, H-70065
1,2,3,9,10,10*a*-Hexahydrophenanthrene, H-80063
1,2,3,6,7,8-Hexahydro-4,5-phenanthrenedione, H-80064
2,3,4,5,6,7-Hexahydro-1,8-phenanthrenedione, H-80065
Hexahydrophthalide, *see* H-70061
Hexahydro-6,1,3[1]-propan[3]ylidene-1*H*-cyclopenta[*c*]triazirino[*a*]pyrazole, *see* T-70205
3,4,4*a*,5,6,7-Hexahydro-2*H*-pyrano[2,3-*b*]pyrilium, H-60055
Hexahydro-2,5-pyrazinedicarboxylic acid, *see* P-60157
Hexahydro-1*H*-pyrazolo[1,2-*a*]pyridazine, H-70067
1,2,3,6,7,8-Hexahydropyrene, H-70069
1,2,3,3*a*,4,5-Hexahydropyrene, H-70068
as-Hexahydropyrene, *see* H-70068
s-Hexahydropyrene, *see* H-70069
Hexahydropyridazino[1,2-*a*]pyridazine-1,4-dione, H-70070
4,5,6,8,9,10-Hexahydropyrido[3,4,5-*ij*]quinolizine, *see* T-60086
Hexahydropyrimidine, H-60056
1,2,3,5,6,7-Hexahydropyrrolizinium(1+), H-70071
Hexahydro-1*H*-pyrrolizin-1-one, H-60057
Hexahydro-3*H*-pyrrolizin-3-one, H-60058
1,2,3,5,10,10*a*-Hexahydropyrrolo[1,2-*b*]isoquinoline, H-70072
1,2,3,6,7,9*a*-Hexahydro-4(1*H*)-quinolizinone, H-70074
3,4,6,7,8,9-Hexahydro-2*H*-quinolizin-2-one, H-60059
5,5*a*,6,11,11*a*,12-Hexahydroquinoxalino[2,3-*b*]quinoxaline, H-80066
Hexahydrosalicylic acid, *see* H-70119
Hexahydro-1,3,4,5-tetrahydroxybenzoic acid, *see* Q-70005
4*a*,5,6,7,7*a*,8-Hexahydro-4,4*a*,7,7*a*-tetramethyl-5,8-epoxy-4*H*-indeno[5,6-*b*]furan, *see* P-60155
2,3,4,7,8,8*a*-Hexahydro-3,6,8,8-tetramethyl-1*H*-3*a*,7-methanoazulen-1-ol, *see* B-60112
▷ Hexahydro-*s*-tetrazine-3,6-dione, *see* T-70097
Hexahydro-1,5-thiazonin-6(7*H*)-one, H-70075
2,3,4,5,8,9-Hexahydrothionin, H-70076
6*bH*-2*a*,4*a*,6*a*-Hexahydrotriazacyclopenta[*cd*]pentalene, H-70077
1*H*,4*H*,7*H*,9*bH*-2,3,5,6,8,9-Hexahydro-3*a*,6*a*,9*a*-triazaphenalene, H-70078
Hexahydro-1,3,5-triazine, H-60060
Hexahydro-1,2,4-triazine-3,6-dione, *see* T-60099
1,3,4,8,9,11*b*-Hexahydro-5,7,11-trihydroxy-4,4,8,11*b*-tetramethylphenanthro[3,2-*b*]furan-6(2*H*)-one, *see* L-70046
4,5,5*a*,6,7,9*a*-Hexahydro-5*a*,6,9*a*-trimethylnaphtho[1,2-*b*]furan, *see* H-60027
1,2,6,7,8,9-Hexahydro-1,6,6-trimethylphenanthro[1,2-*b*]furan-10,11-dione, *see* C-60173
▷ Hexahydro-1,3,5-trimethyl-1,3,5-triazine, *in* H-60060
2,3,6,7,10,11-Hexahydrotrisimidazo[1,2-*a*;1′,2′-*c*;1″,2″-*e*][1,3,5]-triazine, H-60061
3,3′,4,4′,5,5′-Hexahydroxybibenzyl, H-60062
▷ 2,3,14,20,22,25-Hexahydroxy-7-cholesten-6-one, H-60063
2β,3β,14α,20ξ,22ξ,24ξ-Hexahydroxy-5β-cholest-7-en-6-one, *see* P-60192
1α,4β,6β,8β,9α,14-Hexahydroxydihydro-β-agarofuran, *see* E-60018
2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-[1,1′-bianthracene]-9,9′,10,10′-tetrone, *see* R-80007
2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-[1,1′-bianthracene]-9,9′,10,10′-tetrone, *see* R-80008
2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-1,1′-bianthraquinone, *see* R-80007
2,4,4′,5,5′,8′-Hexahydroxy-7,7′-dimethyl-1,1′-bianthraquinone, *see* R-80008
▷ 1,1′,6,6′,7,7′-Hexahydroxy-3,3′-dimethyl-5,5′-bis(1-methylethyl)-[2,2′-binaphthalene]-8,8′-dicarboxaldehyde, *see* G-60032
2′,3,3′,5,7,8-Hexahydroxyflavone, H-70079
2′,3,5,5′,6,7-Hexahydroxyflavone, H-60064
2′,3,5,5′,7,8-Hexahydroxyflavone, H-70080
3,3′,4′,5,6,7-Hexahydroxyflavone, H-80067
3′,4′,5,5′,6,7-Hexahydroxyflavone, H-70081
2′,3′,4′,6,7,8-Hexahydroxyisoflavan, H-80068
2′,4′,5,5′,6,7-Hexahydroxyisoflavone, H-80069
2′,4′,5,5′,7,8-Hexahydroxyisoflavone, H-80070
3′,4′,5,5′,6,7-Hexahydroxyisoflavone, H-80071
2,3,5,6,7,8-Hexahydroxy-1,4-naphthalenedione, *see* H-60065
Hexahydroxy-1,4-naphthoquinone, H-60065
1,2,3,5,6,7-Hexahydroxyphenanthrene, H-60066
2,3,4,8,9,10-Hexahydroxypterocarpan, H-80072
2,3,3′,4,4′,5′-Hexahydroxystilbene, *see* T-60344
Hexaketocyclohexane, *see* C-60210
Hexakis(bromomethylene)cyclohexane, H-80073
Hexakis(dichloromethyl)benzene, H-60067
Hexakis(diethylamino)benzene, *in* B-80014
Hexakis(dimethylamino)benzene, *in* B-80014
3,3′,4′,5,6,7-Hexamethoxyflavone, *in* H-80067
3′,4′,5,5′,6,7-Hexamethoxyflavone, *in* H-70081
2′,3′,4′,6,7,8-Hexamethoxyisoflavan, *in* H-80068
1,1,2,2,4,4-Hexamethyl-3,5-bis(methylene)cyclopentane, H-70082
2,2,3,3,4,4-Hexamethylcyclobutanol, H-60068
Hexamethylcyclobutanone, H-60069
1,1,2,2,3,3-Hexamethylcyclohexane, H-60070

3,3,4,4,5,5-Hexamethyl-1,2-cyclopentanedione, H-80074
Hexamethylene diperoxide diamine, *see* T-70144
Hexamethylene disulfide, *see* D-50815
Hexamethylglutaric acid, *see* H-80076
2,2,3,4,5,5-Hexamethyl-3-hexene, H-70083
1,1,2,2,3,3-Hexamethylindane, H-80075
2,2,3,3,4,4-Hexamethylpentane, H-60071
Hexamethylpentanedioic acid, H-80076
Hexamethylquercetagenin, *in* H-80067
3,7,11,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaen-1-ol, H-80077
3,3,4,4,5,5-Hexamethyltetrahydropyran-2,6-dione, *see* D-80210
2-[3,7,11,15,19,23-Hexamethyl-25-(2,6,6-trimethyl-2-cyclohexenyl)pentacosa-2,14,18,22-tetraenyl]-3-methyl-1,4-naphthoquinone, H-70084
1,1,3,3,5,5-Hexamethyl-2,4,6-tris(methylene)cyclohexane, H-60072
1,1′,1″-(1,3,6-Hexanetriyl)trisbenzene, *see* T-60386
▷ Hexanicotinoylinositol, *in* I-80015
2,2′,4,4′,6,6′-Hexanitro-[1,1′-biphenyl]-3,3′,5,5′-tetramine, *see* T-60014
[3.3.3.3.3.3]Hexannulane, *see* H-80017
1,4,7,10,25,28,31,34-Hexaoxa[10.10](9,10)anthracenophane, H-70085
1,4,7,22,25,28-Hexaoxa[7.7](9,10)anthracenophane, H-70086
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1,4,7,10,13,16-Hexathiacyclooctadecane, H-70087
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▷ 1,3,5-Hexatriynylbenzene, *see* P-80105
▷ 2-Hexenal, H-60076
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▷ 5-Hexyldihydro-2(3*H*)-furanone, H-60078
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1-(Hexylethenyl)benzene, *see* P-80108
2-Hexyl-5-methyl-3(2*H*)furanone, H-60079
2-Hexyl-5-methyl-3-oxo-2*H*-furan, *see* H-60079
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5-Hexyne-1,4-diamine, H-60080
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5-(4-Hydroxy-3-acetoxy-1-butynyl)-2,2′-bithienyl, *in* B-80166
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3-(Hydroxyacetyl)pyridine, H-70102
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8-Hydroxyachillin, H-60100
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ent-16α-Hydroxy-18-atisanoic acid, *in* A-80184
2-Hydroxy-4-azabenzimidazole, *see* D-60249
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4-Hydroxybenzenemethanol, *see* H-80114

▷ 1-Hydroxy-1,2-benziodoxol-3(1*H*)-one, H-60102
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7-Hydroxy-1,3-benzodioxole-4-carboxylic acid, *see* H-60179
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4-Hydroxybenzofuran, H-70106
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4-Hydroxy-3(2*H*)-benzofuranone, H-80108
5-Hydroxy-3(2*H*)-benzofuranone, H-80109
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5-(6-Hydroxy-2-benzofuranyl)-1,3-benzenediol, *see* M-60146
5-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-7-ol, *see* M-60144
7-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, *see* M-60143
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1-(4-Hydroxy-5-benzofuranyl)-3-phenyl-2-propen-1-one, H-70107
3-(6-Hydroxy-5-benzofuranyl)-2-propenoic acid, H-80113
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4-Hydroxy-2*H*-1-benzothiopyran-2-one, H-70110
2-Hydroxy-4*H*-1-benzothiopyran-4-one, *see* H-70110
2-[(2-Hydroxybenzoyl)amino]-4-methoxybenzoic acid, *see* D-70049
8-*p*-Hydroxybenzoylshiromodiol, *in* S-70039
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4-Hydroxybenzyl alcohol, H-80114
2-Hydroxybenzyl chloride, *see* C-70101
3-Hydroxybenzyl chloride, *see* C-70102
4-Hydroxybenzyl chloride, *see* C-70103
p-Hydroxybenzyl methyl ether, *in* H-80114
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ent-2-Hydroxy-1,15-beyeradien-3-one, H-80115
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ent-7*α*-Hydroxy-15-beyeren-19-oic acid, H-60104
ent-12*β*-Hydroxy-15-beyeren-19-oic acid, H-60105
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2′-Hydroxybiochanin A, *in* T-80106
4′-Hydroxy-2-biphenylcarboxylic acid, H-70111
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2′-Hydroxy-2,4′-bipyridine, H-80118
2-Hydroxy-3,3′-bipyridine, H-80119
2-Hydroxy-4,4′-bipyridine, H-80120
4-Hydroxy-2,2′-bipyridine, H-80121
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5-Hydroxy-2,2′-bipyridine, H-80123
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6-Hydroxy-2,2′-bipyridine, H-80126
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6-Hydroxy-3,3′-bipyridine, H-80129
6-Hydroxy-3,4′-bipyridine, H-80130
11-Hydroxy-2,7(14)-bisaboladien-4-one, H-80131
10-Hydroxy-2,7(14),11-bisabolatrien-4-one, H-80132
6-Hydroxy-2,7,10-bisabolatrien-9-one, H-60107
3-[4-Hydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-(4-hydroxyphenyl)-2-propen-1-one, *see* A-80010
6*a*-Hydroxy-3,4:8,9-bis(methylenedioxy)pterocarpan, *in* P-80053
2-Hydroxy-14,15-bisnor-7-labden-13-one, H-80133
5-Hydroxyborneol, *see* T-70280
5-Hydroxybowdichione, *in* B-70175
12-Hydroxybromosphaerol, H-60108
2-Hydroxybutanal, H-70112
3-Hydroxy-4-butanolide, *see* D-60242
▷ 2-Hydroxy-3-butenenitrile, *in* P-70119
4-Hydroxy-2-butenoic acid, H-80134
2-Hydroxy-4-*tert*-butylcyclopentanecarboxylic acid, H-70113
4-Hydroxy-2-butynophenone, *see* H-80233
5-(4-Hydroxy-1-butynyl)-2,2′-bithiophene, *see* B-80167
α-Hydroxybutyraldehyde, *see* H-70112
2-Hydroxy-*γ*-butyrolactone, *see* D-80212
β-Hydroxy-*γ*-butyrotrimethylbetaine, *see* C-70024
12-Hydroxy-4,11(13)-cadinadien-15-oic acid, H-80135
4-Hydroxy-1,9-cadinadien-3-one, H-80136
8-Hydroxy-1(6),2,4,7(11)-cadinatetraen-12,8-olide, H-70114
12-Hydroxy-4-cadinen-15-oic acid, *in* H-80135
6-Hydroxycaespitol, *in* C-80005
1-Hydroxycarbazole, H-80137
2-Hydroxycarbazole, H-60109
α-Hydroxy-*β*-carboxyisocaproic acid, *see* H-60166
β-Hydroxy-*β*-carboxyisocaproic acid, *see* H-60165
3-Hydroxy-*β*,*β*-carotene-4,4′-dione, *see* A-70066
5-Hydroxycarvacrol, *see* I-60125
2‴-Hydroxychlorothricin, *in* C-60137
11-Hydroxy-3,6-cholestanedione, H-80138
(25*R*)-26-Hydroxycholesterol, *in* C-60147
(25*S*)-26-Hydroxycholesterol, *in* C-60147
2-Hydroxychroman, *see* D-60198
3-Hydroxychroman, *see* D-60199
4-Hydroxychroman, *see* D-60200
5-Hydroxychroman, *see* D-60201
6-Hydroxychroman, *see* D-70175
7-Hydroxychroman, *see* D-60202
8-Hydroxychroman, *see* D-60203
2-Hydroxychrysophanol, *see* T-80322
2-Hydroxy-1,4-cineole, H-80139
3′-Hydroxycinerubin *X*, *see* C-70176
p-Hydroxycinnamaldehyde, *see* H-60213
▷ *p*-Hydroxycinnamic acid, *see* H-80242
9*α*-Hydroxycinnamolide, *in* C-80133
p-Hydroxycinnamoylferuloylmethane, *in* C-80165
14-Hydroxy-8,12-cleistanthadiene-7,11-dione, H-80140
7-Hydroxy-13(17),15-cleistanthadien-18-oic acid, H-70115
11-Hydroxy-8,11,13-cleistanthatrien-7-one, H-80141
7-Hydroxy-3,13-clerodadiene-16,15;18,19-diolide, H-70116
ent-2*α*-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide, H-80142
ent-7*β*-Hydroxy-3,13-clerodadiene-15,16;18,19-diolide, H-70117
ent-7*β*-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide, H-80143
ent-7*α*-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80143
ent-2*α*-Hydroxy-3,13-clerodadien-15-oic acid, H-80144
16-Hydroxy-3,13-clerodadien-15,16-olide, H-70118
ent-2*α*-Hydroxy-3,13-clerodadien-15,16-olide, H-80145
ent-7*β*-Hydroxy-3-clerodene-15,16:18,19-diolide, *in* H-70117
ent-4*β*-Hydroxy-13-cleroden-15-oic acid, *in* C-80142
10*α*-Hydroxycolumbin, *in* C-60160
8*β*-Hydroxycolumbin, *in* C-60160
7-Hydroxy-8(17),13-corymbidienolide, H-60110
2-Hydroxy-3-coumaranone, *see* H-80107
4-Hydroxy-3-coumaranone, *see* H-80108
5-Hydroxy-3-coumaranone, *see* H-80109
6-Hydroxy-3-coumaranone, *see* H-80110
7-Hydroxy-3-coumaranone, *see* H-80111
6-Hydroxycoumarin, *see* H-70109
4-Hydroxycrotonic acid, *see* H-80134
5*β*-Hydroxycrustecdysone, *in* H-60023
5′-Hydroxycudraflavone *A*, *in* C-70205
11*α*-Hydroxycurvularin, *in* C-80166
11*β*-Hydroxycurvularin, *in* C-80166
8*β*-Hydroxycycloaraneosene, *in* C-80170
▷ *N*-Hydroxycyclohexanamine, *see* C-70228
α-Hydroxycyclohexaneacetic acid, *see* C-60212
2-Hydroxycyclohexaneacetic acid lactone, *see* H-70049
2-Hydroxycyclohexanecarboxylic acid, H-70119
2-Hydroxycyclohexanemethanol, H-70120
1-Hydroxy-3-cyclohexene-1-carboxaldehyde, H-80146
2-(2-Hydroxycyclohexyl)propenoic acid lactone, *see* H-70062
10′-Hydroxycyclolycoserone, *in* C-70229
6-Hydroxycyclonerolidol, H-60111
2-Hydroxycyclononanone, H-60112
3-Hydroxycyclononanone, H-60113
2-Hydroxycyclooctanecarboxylic acid, H-70121
2-Hydroxycyclopentanone, H-60114
3-Hydroxycyclopentanone, H-60115
4-Hydroxy-2-cyclopentenone, H-60116
1-Hydroxycyclopropanecarboxylic acid, H-60117
12-Hydroxy-*α*-cyperone, *in* E-80081
5-Hydroxycystofuranoquinol, *in* C-70260
2′-Hydroxydaidzein, *see* T-80306
3′-Hydroxydaidzein, *see* T-80308
8-Hydroxydatriscetin, *see* P-70029
6-Hydroxy-3-deazapurine, *see* H-60157
1-Hydroxydebneyol, *in* D-70010
8-Hydroxydebneyol, *in* D-70010
6-Hydroxydecanoic acid, H-80147
7-Hydroxydecanoic acid, H-80148
9-Hydroxydecanoic acid, H-80149
▷ 4-Hydroxydecanoic acid lactone, *see* H-60078
8-Hydroxy-2-decene-4,6-diynoic acid, H-80150
Hydroxydeguelin, *see* T-80009
3-Hydroxy-1,2-dehydrocostic acid, *see* H-80164
4′-Hydroxydehydrokawain, H-70122
15-Hydroxy-3-dehydrotifruticin, *in* T-80197
8*β*-Hydroxydehydrozaluzanin *C*, *in* Z-60001
3*β*-Hydroxydemethylcryptojaponol, *in* T-60314
4-Hydroxydemethylmedicarpin, *see* T-80336
7*α*-Hydroxy-3-deoxyzaluzanin *C*, *in* Z-60001
3*α*-Hydroxydesoxoachalensolide, *in* H-70135
3*β*-Hydroxydesoxoachalensolide, *in* H-70135
4-Hydroxy-25-desoxyneorollinicin, H-80151
10-Hydroxydibenz[*a,c*]anthracene, *see* B-80050
11-Hydroxydibenz[*a,c*]anthracene, *see* B-80051
1-Hydroxydibenz[*a,c*]anthracene, *see* B-80046

2-Hydroxydibenz[*a,c*]anthracene, *see* B-80047
3-Hydroxydibenz[*a,c*]anthracene, *see* B-80048
4-Hydroxydibenz[*a,c*]anthracene, *see* B-80049
Hydroxydictyodial, *in* D-70145
11β-Hydroxy-11,13-dihydro-8-*epi-confertin*, *in* D-60211
2α-Hydroxy-11α,13-dihydroalantolactone, *in* H-80165
2α-Hydroxy-11β,13-dihydroalantolactone, *in* H-80165
1-Hydroxy-1,3-dihydrobenzofuran, *see* H-60171
2α-Hydroxy-11α,13-dihydroconfertin, *in* D-60211
2′-Hydroxydihydrodaidzein, *see* T-80303
3β-Hydroxy-11β,13-dihydrodesoxoachalensolide, *in* H-70135
14-Hydroxy-11,13-dihydrohypocretenolide, *in* H-70235
3α-Hydroxy-14,15-dihydromanoyl oxide, *in* E-70021
2α-Hydroxydihydroparthenolide, *in* D-70239
9α-Hydroxydihydroparthenolide, *in* D-70239
7-Hydroxy-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazole, H-60118
2-Hydroxy-6-(3,4-dihydroxy-1-pentenyl)benzyl alcohol, *see* S-70056
7-Hydroxy-4-(3,4-dihydroxyphenyl)-2′,5-oxidocoumarin, *see* T-70273
5-Hydroxy-4′,7-dihydroxy-6-rhamnosylisoflavone, *see* I-80098
9α-Hydroxy-11β,13-dihydrozaluzanin *C*, *in* Z-60001
9β-Hydroxy-11β,13-dihydrozaluzanin *C*, *in* D-70305
8α-Hydroxy-11α,13-dihydrozaluzanin*C*, *in* Z-60001
9α-Hydroxy-11β,13-dihyrosantamarine, *in* S-60007
2′-Hydroxy-4′,6′-dimethoxyacetophenone, *in* T-70248
▷ 4′-Hydroxy-3′,5′-dimethoxyacetophenone, *in* T-60315
5-Hydroxy-2,3-dimethoxybenzoic acid, *in* T-70250
2-Hydroxy-4,6-dimethoxybenzophenone, *in* T-80285
4-Hydroxy-2,6-dimethoxybenzophenone, *in* T-80285
5-Hydroxy-6,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287
6-Hydroxy-5,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287
7-Hydroxy-5,6-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287
8-Hydroxy-5,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80288
3-Hydroxy-3′,4-dimethoxybibenzyl, *in* T-60316
4-Hydroxy-3,5-dimethoxybiphenyl, *in* B-80129
2′-Hydroxy-4′,6′-dimethoxychalcone, *in* P-80139
5-Hydroxy-6,7-dimethoxycoumarin, *in* T-80287
6-Hydroxy-5,7-dimethoxycoumarin, *in* T-80287
7-Hydroxy-5,6-dimethoxycoumarin, *in* T-80287
8-Hydroxy-5,7-dimethoxycoumarin, *in* T-80288
3-Hydroxy-7,9-dimethoxycoumestan, *in* T-80294
3-Hydroxy-8,9-dimethoxycoumestan, *in* T-80295
7-Hydroxy-10,12-dimethoxycoumestan, *in* T-80294
7-Hydroxy-11,12-dimethoxycoumestan (obsol.), *in* T-80295
4-Hydroxy-3,6-dimethoxy-1,2-dimethylcarbazole, *in* T-70253
4′-Hydroxy-3′,7-dimethoxyflavan, *in* T-70260
4′-Hydroxy-3′,7-dimethoxyflavone, *in* T-80308
5-Hydroxy-6,7-dimethoxyflavone, *in* T-60322
5-Hydroxy-7,8-dimethoxyflavone, *in* T-60321
2′-Hydroxy-4′,7-dimethoxyisoflavan, *in* T-80302
4′-Hydroxy-2′,7-dimethoxyisoflavan, *in* T-80302
7-Hydroxy-2′,4′-dimethoxyisoflavan, *in* T-80302
2′-Hydroxy-4′,7-dimethoxyisoflavanone, *in* T-80303
7-Hydroxy-2′,4′-dimethoxyisoflavanone, *in* T-80303
7-Hydroxy-3′,4′-dimethoxyisoflavanquinone, *see* P-80018
6-Hydroxy-4′,7-dimethoxyisoflavone, *in* T-80310
7-Hydroxy-3′,4′-dimethoxyisoflavone, *in* T-80308
7-Hydroxy-4′,5-dimethoxyisoflavone, *in* T-80309
7-Hydroxy-4′,8-dimethoxyisoflavone, *in* T-80311
2′-Hydroxy-4′,6′-dimethoxy-3′-methylacetophenone, *in* T-80321
3-Hydroxy-4,6-dimethoxy-2-methylbenzoic acid, *in* T-80324
4-Hydroxy-3,6-dimethoxy-2-methyl-9*H*-carbazole-1-carboxaldehyde, *in* H-70154
4′-Hydroxy-3′,5-dimethoxy-3,4-methylenedioxybibenzyl, *in* P-60044
2-Hydroxy-1,3-dimethoxy-8,9-methylenedioxycoumestan, *in* P-80029
3′-Hydroxy-4′,5-dimethoxy-6,7-methylenedioxyiosflavone, *in* P-80043
6-Hydroxy-2′,7-dimethoxy-4′,5′-methylenedioxyisoflavone, *in* P-80042
7-Hydroxy-2′,6-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80042
7-Hydroxy-5,6-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-70032
7-Hydroxy-5,6-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80043
7-Hydroxy-5,8-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80045
▷ 4-Hydroxy-6,7-dimethoxy-9-(3,4-methylenedioxyphenyl)naphtho[2,3-*c*]-furan-1(3*H*)-one, *see* D-60493
6*a*-Hydroxy-2,3-dimethoxy-8,9-methylenedioxypterocarpan, *in* P-80052
5-Hydroxy-4′,7-dimethoxy-6-methylflavone, *in* T-80326
2-Hydroxy-3,7-dimethoxyphenanthrene, *in* T-60339
2-(3-Hydroxy-2,4-dimethoxyphenyl)-6-benzofuranol, *in* H-80260
2-(4-Hydroxy-2,3-dimethoxyphenyl)-6-benzofuranol, *in* H-80260
1-(2-Hydroxy-4,6-dimethoxyphenyl)-2-buten-1-one, *in* T-80331
▷ 1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone, *in* T-60315
4-(2-Hydroxy-4,6-dimethoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* H-80243
1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[2-methoxy-4-(1-propenyl)phenoxy]-1-propanol, *in* A-80046
1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
3-(4-Hydroxy-3,5-dimethoxyphenyl)propanal, *in* T-80333
3-(4-Hydroxy-3,5-dimethoxyphenyl)-2-propen-1-ol, *see* S-70046
6*a*-Hydroxy-3,9-dimethoxypterocarpan, *in* T-80337
3-Hydroxy-2,9-dimethoxypterocarpan, *in* T-80335
3-Hydroxy-4,9-dimethoxypterocarpan, *in* T-80336
3-Hydroxy-9,10-dimethoxypterocarpan, *in* T-80338
4-Hydroxy-3,9-dimethoxypterocarpan, *in* T-80336
9-Hydroxy-2,3-dimethoxypterocarpan, *in* T-80335
1-Hydroxy-3,7-dimethoxyxanthone, *in* T-80347
1-Hydroxy-5,6-dimethoxyxanthone, *in* T-60349
7-Hydroxy-3,4-dimethyl-2*H*-1-benzopyran-2-one, H-60119
1-(5-Hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-(4-hydroxy-3-methoxyphenyl)-2-propen-1-one, *see* P-80168
7-Hydroxy-2′,2′-dimethyl-[2,6′-bi-2*H*-1-benzopyran]-4(3*H*)one, *see* A-80006
6-(4-Hydroxy-1,3-dimethyl-2-butenylamino)purine, *see* M-60133
7-Hydroxy-3,4-dimethylcoumarin, *see* H-60119
12-Hydroxy-6,14-dimethyl-1,7-dioxacyclotetradeca-3,9-diene-2,8,11-trione, *in* C-60159
4-Hydroxy-2,5-dimethyl-3(2*H*)-furanone, H-60120
3-Hydroxy-10,10-dimethyl-6*H*,10*H*-furo[3,2-*c*:4,5-*g*′]bis[1]benzopyran-6-one, *see* S-80038
6-Hydroxy-2,4-dimethylheptanoic acid, H-60121
5-Hydroxy-8,8-dimethyl-6-(3-methyl-2-butenyl)-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *see* H-70093
7-Hydroxy-2,2′-dimethyl-8′-(3-methyl-2-butenyl)-[2,6′-bi-2*H*-1-benzopyran]-4(3*H*)one, *see* A-80008
5-Hydroxy-2,2-dimethyl-6-(3,4-methylenedioxystyryl)chromene, *see* G-70014
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *in* M-80001
5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *in* M-80001
5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *in* M-80001
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *see* M-80001
6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3*H*,9*H*-[1,2]-dioxolo[3′,4′:4,5]furo[2,3-*f*][1]benzopyran-3-one, H-80152
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*,3,4-*b*′]dipyran-2-one, *in* M-80001
3-(2-Hydroxy-4,8-dimethyl-3,7-nonadienyl)benzaldehyde, H-60122
2-(3-Hydroxy-3,7-dimethyl-2,6-octadienyl)-1,4-benzenediol, *in* H-80153
2-(3-Hydroxy-3,7-dimethyl-6-octenyl)-1,4-benzenediol, H-80153
2-(7-Hydroxy-3,7-dimethyl-2-octenyl)-6-methoxy-1,4-benzoquinone, H-60123
4-Hydroxy-3,3-dimethyl-2-oxobutanoic acid, H-60124
5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *in* M-80001
3-Hydroxy-4,4-dimethyl-2-pentanone, H-80154
2-Hydroxy-1,3-dimethyl-5*H*-phenanthro[4,5-*bcd*]pyran-5-one, *see* S-80006
α-Hydroxy-2,6-dinitrotoluene, *see* D-60459
15-Hydroxy-12,19-dioxo-13,14-dehydro-10,11,14,15-tetrahydrogeranylnerol, *in* H-60186
5-Hydroxy-1,7-diphenyl-3-heptanone, *in* D-70481
5-Hydroxy-1,7-diphenyl-1-hepten-3-one, *in* D-70481
5-Hydroxy-5,5-diphenylpentanoic acid, H-80155
2-Hydroxy-1,2-diphenyl-1-propanone, H-70123

2-Hydroxy-1,3-diphenyl-1-propanone, H-70124
10-Hydroxy-7,11,13,16,19-docosapentaenoic acid, H-70125
Hydroxydodecahedrane, *see* D-80523
11-Hydroxydodecanoic acid, H-80157
7-Hydroxydodecanoic acid, H-80156
2-Hydroxy-2-dodecenal, *see* O-70087
10-Hydroxy-11-dodecenoic acid, H-60125
12-Hydroxy-10-dodecenoic acid, H-60126
7-*O*-(3-Hydroxy-7-drimen-11-yl)isofraxidin, H-80158
20-Hydroxyecdysone, *in* H-60063
3-*epi*-20-Hydroxyecdysone, *in* H-60063
5β-Hydroxyecdysterone, *in* H-60023
19-Hydroxyeicosanoic acid, *see* H-80176
8-Hydroxy-5,9,11,14,17-eicosapentaenoic acid, H-70126
12-Hydroxy-5,8,10,14-eicosatetraenoic acid, H-60131
5-Hydroxy-6,8,11,14-eicosatetraenoic acid, H-60127
8-Hydroxy-5,9,11,14-eicosatetraenoic acid, H-60128
20-Hydroxyelemajurinelloide, H-60132
6α-Hydroxy-8-epiivangustin, *in* I-70109
10′-Hydroxy-1′-epilycoserone, *in* L-70045
ent-16-Hydroxy-13-epimanoyl oxide, *in* E-70023
12α-Hydroxy-13-epi-manoyl oxide, *in* E-70023
2β-Hydroxy-3,4-epoxyjaeschkeanadiol, *in* E-80022
11-Hydroxy-12,13-epoxy-9,15-octadecadienoic acid, H-70127
10-Hydroxy-1,11(13)-eremophiladien-12,8-olide, H-80159
5-Hydroxyerythrinin *A*, *see* A-80050
▷ *N*-Hydroxyethanimidamide, *see* A-60016
1-(2-Hydroxyethyl)-1,4-cyclohexanediol, H-60133
6-(1-Hydroxyethyl)-7,8-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran, *in* A-80023
6-(1-Hydroxyethyl)eupatoriochromene *B*, *in* A-80023
O-(2-Hydroxyethyl)hydroxylamine, H-60134
5-(1-Hydroxyethyl)-2-(1-hydroxy-1-methylethyl)benzofuran, *in* A-70044
α-Hydroxy-1-ethylnaphthalene, *see* N-70015
3-(2-Hydroxyethyl)piperidine, *see* P-70103
2-(1-Hydroxyethyl)thiophene, *see* T-80178
3-(1-Hydroxyethyl)thiophene, *see* T-80179
3-(2-Hydroxyethyl)thiophene, *see* T-60211
2-Hydroxy-4,11(13)-eudesmadien-15-al, H-80160
9-Hydroxy-4,11(13)-eudesmadien-12-oic acid, H-60135
15-Hydroxy-4,11(13)-eudesmadien-12,8-olide, H-60138
2-Hydroxy-3,11(13)-eudesmadien-12,8-olide, H-80161
3-Hydroxy-4,11(13)-eudesmadien-12,8-olide, H-60136
7-Hydroxy-4,11(13)-eudesmadien-12,6-olide, H-70128
7-Hydroxy-4,11(13)-eudesmadien-12,6-olide, H-80162
9-Hydroxy-4,11(13)-eudesmadien-12,6-olide, H-60137
1β-Hydroxy-3,11(13)-eudesmadien-12,6α-olide, *see* S-60007
1β-Hydroxy-4,11(13)-eudesmadien-12,8β-olide, *see* I-70109
6-Hydroxy-1,4-eudesmadien-3-one, H-60139
12-Hydroxy-4,11(13)-eudesmadien-3-one, *in* E-80081
2-Hydroxy-1,4,6-eudesmatriene-3,8-dione, H-80163
3-Hydroxy-1,4(15),11(13)-eudesmatrien-12-oic acid, H-80164
1-Hydroxy-2,4(15),11(13)-eudesmatrien-12,8-olide, H-70129
1-Hydroxy-3,7(11),8-eudesmatrien-12,8-olide, H-60140
1-Hydroxy-4(15),7(11),8-eudesmatrien-12,8-olide, H-60141
2-Hydroxy-5-eudesmen-12,8-olide, H-80165
3-Hydroxy-4-eudesmen-12,8-olide, H-80166
4-Hydroxy-11(13)-eudesmen-12,8-olide, H-60142
18-Hydroxyferruginol, *see* A-70005
6-Hydroxyflavone, H-70130
7-Hydroxyflavone, H-70131
▷ 8-Hydroxyflavone, H-70132
2-Hydroxyflemichapparin C, *in* T-80088
1-Hydroxyfluorene, *see* F-80016
2′-Hydroxyformononetin, *in* T-80306
3β-Hydroxy-27-friedelanal, *see* T-70218
27-Hydroxy-3,21-friedelanedione, *in* D-70301
3α-Hydroxy-27-friedelanoic acid, *in* T-70218
3β-Hydroxy-27-friedelanoic acid, *in* T-70218
27-Hydroxy-3-friedelanone, *in* D-70301
3-Hydroxy-D-friedoolean-14-en-28-oic acid, *see* H-80256
7-Hydroxyfrullanolide, *in* H-80162
▷ 9-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, *see* X-60002
10-Hydroxy-2*H*,13*H*-furo[3,2-*c*:5,4-*h*′]bis[1]benzopyran-2,13-dione, H-70133
4-Hydroxyfuro[2,3-*d*]pyridazine, H-60146
7-Hydroxyfuro[2,3-*d*]pyridazine, H-60147
2-Hydroxygarveatin *A*, *in* H-60148
2-Hydroxygarveatin *B*, H-60148
2-Hydroxygarvin *B*, *in* G-60009
6α-Hydroxygedunin, *in* G-70006
2′-Hydroxygenistein, *see* T-80106
6-Hydroxygenistein, *see* T-80112
6-Hydroxy-1(10),4,11(13)-germacratrien-12,8-olide, H-70134
3β-Hydroxy-1(10),4,11(13)-germacratrien-12,6α-olide, *see* H-60006
4-Hydroxyglutamic acid, *see* A-60195
4-Hydroxygrenoblone, *in* G-70029
15-Hydroxy-3,10(14)-guaiadien-12,8-olide, H-70136
3-Hydroxy-4,11(13)-guaiadien-12,8-olide, H-70135
4-Hydroxy-1(10),11(13)-guaiadien-12,8-olide, H-80167
10α-Hydroxy-3,11(13)-guaiadien-12,6α-olide, *see* C-80164
5-Hydroxy-3,11(13)-guaiatrien-12,8-olide, H-70137
8-Hydroxy-4(15),11(13),10(14)-guaiatrien-12,6-olide, H-70138
4-Hydroxy-10(14)-guaien-12,8-olide, H-80168
4-Hydroxy-9-guaien-12,8-olide, H-80169
3β-Hydroxy-4-guaien-12,8β-olide, *in* H-70135
11-Hydroxy-4-guaien-3-one, H-60149
8-Hydroxyguanosine, *see* D-70238
17-Hydroxygutiesolbriolide, *in* G-80045
9α-Hydroxygymnomitryl acetate, *in* G-70035
9α-Hydroxygymnomitryl cinnamate, *in* G-70035
2α-Hydroxyhanphyllin-3-*O*-acetate, *in* H-60006
2β-Hydroxyhardwickiic acid, *in* H-70002
2-Hydroxyhautriwaic acid, *in* H-70002
3β-Hydroxyhebeclinolide, *in* H-60009
17-Hydroxyhebemacrophyllide, *in* H-60010
5-Hydroxyhemimellitene, *see* T-60371
10-Hydroxy-16-hentriacontanone, H-80170
8-Hydroxy-5-hentriacontanone, H-80171
5-Hydroxy-3,3′,4′,5′,6,7,8-heptamethoxyflavone, *in* O-70018
5-(1-Hydroxy-2,4,6-heptatriynyl)-2-oxo-1,3-dioxolane-4-heptanoic acid, *see* A-70224
3-(7-Hydroxy-5-heptene-1,3-diynyl)phenol, *see* H-80234
7-Hydroxy-5-heptynoic acid, H-60150
11-Hydroxyhexadecanoic acid, H-80172
15-Hydroxyhexadecanoic acid, H-80173
16-Hydroxy-9-hexadecenoic acid o-lactone, *see* I-60086
3-Hydroxy-3′,4′,5,6,7,8-hexamethoxyflavone, *in* H-80028
3′-Hydroxy-4′,5,5′,6,7,8-hexamethoxyflavone, *in* H-80029
4′-Hydroxy-3′,5,5′,6,7,8-hexamethoxyflavone, *in* H-80029
5-Hydroxy-3,3′,4′,6,7,8-hexamethoxyflavone, *in* H-80028
5-Hydroxy-3′,4′,5′,6,7,8-hexamethoxyflavone, *in* H-80029
3-Hydroxy-5-hexanolide, *see* T-60067
3-Hydroxy-22,23,24,25,26,27-hexanor-20-dammaranone, H-60151
2α-Hydroxyhippuristanol, *in* E-80039
4-Hydroxyhomopterocarpin, *in* T-80336
3-Hydroxyhomotyrosine, *see* A-60185
5-Hydroxyhydantoin, *see* H-60156
6-Hydroxy-2-(*p*-hydroxybenzylidene)-3(2*H*)benzofuranone, *see* D-80273
7-Hydroxy-3-(4-hydroxybenzylidene)-4-chromanone, H-60152
6-Hydroxy-2-(3-hydroxy-2,4-dimethoxyphenyl)benzofuran, *in* H-80260
6-Hydroxy-2-(4-hydroxy-2,3-dimethoxyphenyl)benzofuran, *in* H-80260
7-Hydroxy-1-hydroxy-3,7-dimethyl-2*E*,5*E*-octadien-4-one, *in* D-60318
4-Hydroxy-4-(2-hydroxyethyl)cyclohexanone, H-60153
4-Hydroxy-5-(1-hydroxyethyl)-3-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, *see* M-70091
4-Hydroxy-5-(1-hydroxyethyl)-3-*C*-prenylcoumarin, *see* M-70091
5-Hydroxy-2-[5-hydroxy-2-(hydroxymethyl)-4-pyrimidinyl]-7-methyl-4-benzoxazolecarboxamide, *see* B-70176
5-Hydroxy-6-(4-hydroxy-3-methoxycinnamoyl)-2,2-dimethyl-2*H*-1-benzopyran, *see* P-80168
2-Hydroxy-4-[(2-hydroxy-4-methoxy-3,6-dimethylbenzoyl)oxy]-3,6-dimethylbenzoic acid, *see* B-70007
2-Hydroxy-4-[[2-hydroxy-4-methoxy-6-(2-oxoheptyl)benzoyl]oxy]-6-(2-oxoheptyl)benzoic acid, *see* M-70147
2-Hydroxy-4-[(2-hydroxy-4-methoxy-6-pentylbenzoyl)oxy]-6-pentylbenzoic acid, *see* P-80070
6-Hydroxy-2-(4-hydroxy-2-methoxyphenyl)benzofuran, *in* D-80363
7-Hydroxy-3-(2-hydroxy-4-methoxyphenyl)coumarin, *in* D-80364
5-Hydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-4*H*-1-benzopyran-4-one, *see* D-70291
5-Hydroxy-4-(3-hydroxy-4-methoxyphenyl)-7-methoxycoumarin, *in* D-80356
6-Hydroxy-2-(2-hydroxy-4-methoxyphenyl)-3-methoxy-5-*C*-prenylbenzofuran, *see* A-80057
5-Hydroxy-2-(3-hydroxy-4-methoxyphenyl)-6,7,8-trimethoxy-4*H*-1-benzopyran-4-one, *see* D-60375
6-Hydroxy-2-(5-hydroxy-3-methoxy-2-prenylphenyl)benzofuran, *in* M-60146
2-Hydroxy-4-[(2-hydroxy-4-methoxy-6-propylbenzoyloxy)]-6-pentylbenzoic acid, *see* S-80044
7-Hydroxy-6-(hydroxymethyl)-2*H*-1-benzopyran-2-one, H-70139
2-Hydroxy-4-hydroxymethyl-4-butanolide, *see* D-70212
4-Hydroxy-3-(2-hydroxy-3-methyl-3-butenyl)benzoic acid, H-60154
11-Hydroxy-3-(1-hydroxy-3-methylbutyl)-4-methoxy-9-methyl-5*H*,7*H*-dibenzo[*b*,*g*][1,5]dioxocin-5-one, *see* P-80019
7-Hydroxy-6-hydroxymethylcoumarin, *see* H-70139
1-[3-Hydroxy-4-(hydroxymethyl)cyclopentyl]-2,4(1*H*,3*H*)-pyrimidinedione, H-70140

3-Hydroxy-4-(hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptan-2-one, *in* H-70173
3β-Hydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, *in* L-60036
7-Hydroxy-3-(2-hydroxy-4,5-methylenedioxyphenyl)coumarin, *in* H-80261
10-Hydroxy-2-(6-hydroxy-4-methyl-4-hexylidene)-6,10-dimethyl-7-oxo-8-undecenal, *in* H-60186
3-Hydroxy-2-hydroxymethyl-1-methoxyanthraquinone, *in* D-70306
5-Hydroxy-6-(hydroxymethyl)-7-methoxy-2-methyl-4*H*-1-benzopyran-4-one, H-60155
5-Hydroxy-6-hydroxymethyl-7-methoxy-2-methylchromone, *see* H-60155
1-[5-Hydroxy-2-(hydroxymethyl)-2-methyl-2*H*-1-benzopyran-6-yl]ethanone, *see* A-60031
4-Hydroxy-5-(hydroxymethyl)-3-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, *see* L-60034
12-Hydroxy-6-(hydroxymethyl)-10-methyl-2-(4-methyl-3-pentenyl)-2,6,10-dodecatrienal, *in* H-70179
7-Hydroxy-6-[2-hydroxy-2-(2-methyl-5-oxotetrahydro-2-furyl)ethyl]-5-methoxy-4-methyl-1-phthalanone, *see* H-80175
3-Hydroxy-5-(4-hydroxy-4-methylpentyl)-2-isopropyl-6-methyl-1,4-naphthoquinone, *see* H-80254
3-Hydroxy-5-(4-hydroxy-4-methylpentyl)-6-methyl-2-(1-methylethyl)-1,4-naphthalenedione, *see* H-80254
5-[3-Hydroxy-2-(hydroxymethyl)phenyl]-4-pentene-2,3-diol, *see* S-70056
4-Hydroxy-5-hydroxymethyl-3-prenylcoumarin, *see* L-60034
2-Hydroxy-2-(hydroxymethyl)-2*H*-pyran-3(6*H*)-one, H-70141
2-Hydroxy-5-(7-hydroxy-4-oxo-4*H*-1-benzopyran-3-yl)benzyaldehyde, *see* C-80153
4-Hydroxy-3-(9-hydroxy-8-oxofarnesyl)-5-methylcoumarin, *in* H-70183
4-Hydroxy-α-[3-hydroxy-5-oxo-4-(3,4,5-trihydroxyphenyl)-2(5*H*)-furanylidene]benzeneacetic acid, *see* G-70026
5-Hydroxy-3-(4-hydroxyphenyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, *see* D-80031
5-Hydroxy-7-(4-hydroxyphenyl)-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, *see* A-80050
9-Hydroxy-7-(4-hydroxyphenyl)-8*H*-1,3-dioxolo[4,5-*g*][1]benzopyran-8-one, *see* D-80341
5-Hydroxy-4-(4-hydroxyphenyl)-2(5*H*)-furanone, H-80174
3-Hydroxy-4-(4-hydroxyphenyl)-6-[(4-hydroxyphenylmethylene)]-2*H*-pyran-2,5(6*H*)-dione, *see* G-60038
7-Hydroxy-3-(4-hydroxyphenyl)-5-methoxy-4*H*-1-benzopyran-4-one, *see* D-80336
6-Hydroxy-2-[(4-hydroxyphenyl)methylene]-3(2*H*)-benzofuranone, *see* D-80273
3-Hydroxy-5-(4-hydroxyphenyl)pentanoic acid, H-70142
3-Hydroxy-2-(4-hydroxy-3-*C*-prenylphenyl)-5,6-dimethoxybenzofuran, *see* L-80027
8-Hydroxy-3-(2-hydroxypropyl)-6-methoxy-1*H*-2-benzopyran-1-one, *see* D-80062
8-Hydroxy-3-(2-hydroxypropyl)-6-methoxyisocoumarin, *see* D-80062
7-Hydroxy-6-[2-hydroxy-2-(tetrahydro-2-methyl-5-oxo-2-furyl)ethyl]-5-methoxy-4-methylphthalide,8CI, H-80175
14-Hydroxyhypocretenolide, *in* H-70235
19-Hydroxyicosanoic acid, H-80176
11-Hydroxy-5,8,12,14-icosatetraenoic acid, H-60130
9-Hydroxy-5,7,11,14-icosatetraenoic acid, H-60129
8-Hydroxy-5,9,11,14-icosatetraenoic acid, *in* H-70126
23-Hydroxyimberbic acid, *in* T-80328
15-Hydroxyimbricatolal (incorr.), *in* H-70150
14-Hydroxyimidazo[1,2-*a*: 3,4-*a*′]diquinolin-7-ium hydroxide, inner salt, *see* B-80063
5-Hydroxy-2,4-imidazolidinedione, H-60156
2-Hydroxy-4,5-imidazolidinedione, *see* D-60243
2-Hydroxyimidazo[*b*]pyrazine, *see* I-60006
6-Hydroxyimidazo[4,5-*c*]pyridazine, *see* D-60248
4-Hydroxyimidazo[4,5-*b*]pyridine, H-60157
2-Hydroxyimidazo[*b*]pyridine, *see* D-60249
3-Hydroxyiminoindole, *in* I-60035
▷ 1-Hydroxyindeno[1,2,3-*cd*]pyrene, *see* I-60022
▷ 2-Hydroxyindeno[1,2,3-*cd*]pyrene, *see* I-60023
▷ 6-Hydroxyindeno[1,2,3-*cd*]pyrene, *see* I-60024
▷ 7-Hydroxyindeno[1,2,3-*cd*]pyrene, *see* I-60025
▷ 8-Hydroxyindeno[1,2,3-*cd*]pyrene, *see* I-60026
6-Hydroxyindole, H-60158
6*a*-Hydroxyinermin, *in* T-80121
2-Hydroxy-5-iodobenzaldehyde, H-70143
3-Hydroxy-2-iodo-6-methylpyridine, H-60159
3-[4-(4-Hydroxy-3-iodophenoxy)-3,5-diiodophenyl]alanine, *see* T-60350
O-(4-Hydroxy-3-iodophenyl)-3,5-diiodotyrosine, *see* T-60350
5-Hydroxy-6-iodo-2-picoline, *see* H-60159
3-Hydroxy-2-iodopyridine, H-60160
2-Hydroxyislandicin, *see* T-60112
1α-Hydroxyisoafraglaucolide, *in* I-70060
3α-Hydroxyisoagatholal, *in* D-70310
3β-Hydroxyisoagatholal, *in* D-70310
9α-Hydroxyisoalantolactone, *in* I-80046
9β-Hydroxyisoalantolactone, *in* I-80046
15-Hydroxyisoalloalantolactone, *in* I-80047
5′-Hydroxyisoavrainvilleol, *see* B-70194
4-Hydroxyisobacchasmacranone, H-60161
10α-Hydroxy-6-isodaucen-14-al, *in* O-70093
17-Hydroxyisogutiesolbriolide, *in* I-80062
ent-12β-Hydroxyisokauren-19-oic acid, *see* H-80180
▷ 3-(4-Hydroxy-L-isoleucine)-α-amanitin, *in* A-60084
4′-Hydroxyisolonchocarpin, *in* I-80066
2′-Hydroxyisolupalbigenin, H-80177
10′-Hydroxyisolycoserone, *in* I-70068
6*a*-Hydroxyisomedicarpin, *in* T-80337
1-Hydroxyisoondetianone, *see* H-80263
2-Hydroxyisophthalic acid, *see* H-60101
6α-Hydroxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
7α-Hydroxyisopimara-8(14)15-dien-18-oic acid, *in* S-80008
12β-Hydroxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
3β-Hydroxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
18-Hydroxy-8,15-isopimaradien-7-one, H-60162
8-Hydroxyisopimar-15-ene, H-60163
4-Hydroxy-2-isopropyl-5-benzofurancarboxylic acid, H-60164
2-Hydroxy-2-isopropylbutanedioic acid, H-60165
2-Hydroxy-3-isopropylbutanedioic acid, H-60166
7-Hydroxy-4-isopropyl-3-methoxy-6-methylcoumarin, H-70144
2-Hydroxy-2-isopropylsuccinamic acid, *in* H-60165
2-Hydroxy-2-isopropylsuccinamide, *in* H-60165
2-Hydroxy-2-isopropylsuccinic acid, *see* H-60165
2-Hydroxy-3-isopropylsuccinic acid, *see* H-60166
7-Hydroxy-3-isopropyl-5,5,9-trimethyl-1,2,6(5*H*)-anthracenetrione, *see* P-70144
2′-Hydroxyisoprunetin, *in* T-80106
6-Hydroxyisoquinoline, H-80178
β-Hydroxyisovalerylshikonin, *in* S-70038
4-Hydroxyisovaline, *see* A-60186
2α-Hydroxyivangustin, *in* I-70109
14α-Hydroxyixocarpanolide, *in* I-60143
11-Hydroxyjasionone, *in* J-80003
9″-Hydroxyjasmesoside, *in* J-80004
9″-Hydroxyjasmesosidic acid, *in* J-80004
Hydroxyjavanicin, *see* F-60108
2-Hydroxyjuglone, *see* D-60354
3-Hydroxyjuglone, *see* D-60355
20-Hydroxyjurinelloide, *in* J-60003
ent-19-Hydroxy-16*S*-kauran-17-al, *in* K-70008
ent-1α-Hydroxy-16-kauren-19-oic acid, H-80179
ent-12β-Hydroxy-15-kauren-19-oic acid, H-80180
ent-3β-Hydroxy-15-kauren-17-oic acid, H-60167
ent-3β-Hydroxy-16-kauren-18-oic acid, H-80181
γ-Hydroxy-α-ketobutyric acid, *see* H-80227
15-Hydroxy-8(17),12-labdadien-16-al, H-70145
19-Hydroxy-8(17),13-labdadien-15-al, H-70146
13*R*-Hydroxy-8,14-labdadiene-2,7-dione, *in* D-80327
2-Hydroxy-8(17),13-labdadien-15-oic acid, H-70147
ent-6β-Hydroxy-8(17),13-labdadien-15-oic acid, H-70148
16-Hydroxy-8(17),13-labdadien-15,16-olid-19-oic acid, H-80182
ent-15-Hydroxy-7,13-labdadien-2-one, *in* L-80004
ent-15-Hydroxy-8,13-labdadien-7-one, *in* L-70004
13*R*-Hydroxy-8(17),14-labdadien-3-one, *in* L-70002
ent-6β-Hydroxy-7,12*E*,14-labdatrien-17-oic acid, *in* L-60004
15-Hydroxy-8(17)-labden-19-al, H-70150
8-Hydroxy-13-labden-15-al, H-70149
15-Hydroxy-7-labden-17-oic acid, H-60168
15-Hydroxy-7-labden-17-oic acid, H-80183
15-Hydroxy-7-labden-3-one, H-70151
4-Hydroxylamino-1,2,3-benzotriazine, *in* A-60092
▷ Hydroxylaminocyclohexane, *see* C-70228
4-Hydroxylaminoquinoline, *see* H-80253
3-Hydroxy-8,24-lanostadien-21-oic acid, H-70152
3-Hydroxy-8-lanosten-26,22-olide, H-60169
21-Hydroxylanosterol, *in* L-70017
2α-Hydroxylaurenobiolide, *in* H-70134
Hydroxyleptomycin *A*, *see* K-70007
2-Hydroxyligustrin, H-80184
1-Hydroxylinalool, *in* D-80456
9-Hydroxylinalool, *in* D-80456
23-Hydroxylongispinogenin, *in* O-60035
5-Hydroxy-14,15-LTA$_4$, *see* E-70016
28-Hydroxy-20(29)-lupene-3,7-dione, H-80185
3-Hydroxy-20(29)-lupen-11-one, H-80186
7-Hydroxy-20(29)-lupen-3-one, H-80187
15-Hydroxylycopersene, *in* L-70044
6*a*-Hydroxymaackiain, *in* T-80121
4-Hydroxymaackiain, *in* T-80119
3α-Hydroxymanool, *in* L-70002
19-Hydroxymanoyl oxide, *in* E-70023
6*a*-Hydroxymedicarpin, *in* T-80337
4-Hydroxymedicarpin, *in* T-80336
9α-Hydroxymedioresinol, *in* M-70016
3-Hydroxy-2-mercaptopyridine, *see* H-60222
▷ 2-Hydroxy-3-methoxybenzaldehyde, *in* D-70285
3-Hydroxy-2-methoxybenzaldehyde, *in* D-70285
3-Hydroxy-4-methoxybenzenemethanol, *in* D-80284
4-Hydroxy-3-methoxybenzenemethanol, *in* D-80284
5-(5-Hydroxy-6-methoxy-2-benzofuranyl)-1,3-benzenediol, *in* M-60146

6-Hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, H-80188
▷ 7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, H-80189
3-Hydroxy-4-methoxybenzyl alcohol, *in* D-80284
3-Hydroxy-5-methoxybibenzyl, *in* P-80100
1-Hydroxy-2-methoxybiphenylene, *in* B-80116
3-Hydroxy-3′-methoxy-2,2′-bipyridine, *in* D-80290
6-Hydroxy-4-methoxy-2,2′-bipyridine, *in* D-80296
4*a*-Hydroxy-8-methoxychlorotetracycline, *in* M-70045
4-Hydroxy-3-methoxycinnamaldehyde, *see* C-80148
ent-4α-Hydroxy-3β-methoxy-13-cleroden-15,16-olide, *in* D-80303
6-Hydroxy-7-methoxycoumarin, *see* H-80188
▷ 7-Hydroxy-6-methoxycoumarin, *see* H-80189
3-Hydroxy-5-methoxy-4,4-dimethyl-2-(1-oxo-3-phenyl-2-propenyl)-2,5-cyclohexadien-1-one, *see* C-80038
10-Hydroxy-11-methoxydracaenone, *in* D-70546
1β-Hydroxy-6α-methoxy-4(15)-eudesmene, *in* E-80084
5-Hydroxy-6-methoxyindole, *in* D-70307
6-Hydroxy-5-methoxyindole, *in* D-70307
7-Hydroxy-4′-methoxyisoflavanone, *in* D-80322
▷ 7-Hydroxy-4′-methoxyisoflavone, H-80190
15-Hydroxy-7α-methoxy-8-labden-17-oic acid, *in* D-80330
3-Hydroxy-1-methoxy-2-(methoxymethyl)anthraquinone, *in* D-70306
7-Hydroxy-4-methoxy-5-methyl-2*H*-1-benzopyran-2-one, *in* D-60348
2-Hydroxy-3-methoxy-5-methyl-1,4-benzoquinone, *in* D-70320
3-Hydroxy-2-methoxy-5-methyl-1,4-benzoquinone, *in* D-70320
7-Hydroxy-6-methoxy-8-(3-methyl-2-butenyl)-2*H*-1-benzopyran-1-one, *see* C-60026
4-Hydroxy-3-methoxy-2-methyl-9*H*-carbazole-1-carboxaldehyde, H-70154
7-Hydroxy-4-methoxy-5-methylcoumarin, *in* D-60348
2-Hydroxy-3-methoxy-8,9-methylenedioxycoumestan, *in* T-80088
3-Hydroxy-2-methoxy-8,9-methylenedioxycoumestan, *in* T-80088
3-Hydroxy-4-methoxy-8,9-methylenedioxycoumestan, *in* T-80089
7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavan, *in* T-80097
7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavanone, *in* T-80101
2′-Hydroxy-5-methoxy-6,7-methylenedioxyisoflavone, *in* T-80108
4′-Hydroxy-5-methoxy-6,7-methylenedioxyisoflavone, *in* D-80341
5-Hydroxy-2′-methoxy-6,7-methylenedioxyisoflavone, *in* T-60107
7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavone, *in* T-80107
7-Hydroxy-6-methoxy-3′,4′-methylenedioxyisoflavone, *in* T-80111
7-Hydroxy-8-methoxy-3′,4′-methylenedioxyisoflavone, *in* T-70112
6*a*-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan, *in* T-80121
2-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan, *in* T-80117
3-Hydroxy-4-methoxy-8,9-methylenedioxypterocarpan, *in* T-80119
4-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan, *in* T-80119
3-Hydroxy-6-methoxy-8,9-methylenedioxypterocarpan, *see* S-60038
3-Hydroxy-4-methoxy-8,9-methylenedioxypterocarpene, *in* T-80122
7-Hydroxy-3-methoxy-6-methyl-4-(1-methylethyl)-2*H*-1-benzopyran-2-one, *see* H-70144
6-Hydroxy-7-methoxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran, H-80191
3-Hydroxy-5-methoxy-2-methyl-1,4-naphthoquinone, *in* D-60350
6-Hydroxy-5-methoxy-2-methyl-1,4-naphthoquinone, *in* D-60351
3-Hydroxy-4-methoxy-1-methyl-7-oxabicyclo[4.1.0]hept-3-ene-2,5-dione, *in* D-70320
5-Hydroxy-7-methoxy-6-methylphthalide, *in* D-60349
2-Hydroxy-5-methoxy-1,4-naphthoquinone, *in* D-60354
2-Hydroxy-8-methoxy-1,4-naphthoquinone, *in* D-60355
4-Hydroxy-5-methoxy-2-nitrobenzoic acid, *in* D-60360
5-Hydroxy-4-methoxy-2-nitrobenzoic acid, *in* D-60360
5-Hydroxy-3-methoxy-7-oxabicyclo[4.1.0]hept-3-en-2-one, H-70155
7-Hydroxy-6-methoxy-3-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-2*H*-1-benzopyran-2-one, *see* D-70006
3-Hydroxy-5-methoxy-4-(1-oxo-2,4-octadienyl)benzeneacetic acid, *see* C-60024
2-Hydroxy-5-methoxy-3-(10-pentadecenyl)-1,4-benzoquinone, *see* M-60004
5-Hydroxy-7-methoxy-2-pentyl-4*H*-1-benzopyran-4-one, H-80192
5-Hydroxy-7-methoxy-2-pentylchromone, *see* H-80192
3-Hydroxy-7-methoxy-9-pentyl-1-propyldibenzofuran-2-carboxylic acid, *see* I-60098
3-Hydroxy-4-methoxyphenylacetaldehyde, *in* D-60371
4-Hydroxy-3-methoxyphenylacetaldehyde, *in* D-60371
3-(4-Hydroxy-2-methoxyphenyl)-2*H*-1-benzopyran-7-ol, *in* T-80305
▷ 7-Hydroxy-3-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, *see* H-80190
7-Hydroxy-6-methoxy-4-phenyl-2*H*-1-benzopyran-2-one, *see* I-60097
7-Hydroxy-6-methoxy-4-phenylcoumarin, *see* I-60097
5-[2-(3-Hydroxy-4-methoxyphenyl)ethenyl]-1,3-benzenediol, *in* D-80361
6-[2-(4-Hydroxy-3-methoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one, *in* H-70122
1-(4-Hydroxy-3-methoxyphenyl)-2-(4-hydroxy-3,5-dimethoxyphenyl)-1,3-propanediol, *in* B-80150
2-(2-Hydroxy-4-methoxyphenyl)-5-hydroxy-6-methoxybenzofuran, *see* S-60002
1-(3-Hydroxy-5-methoxyphenyl)-2-(4-hydroxy-3-methoxyphenyl)ethane, *in* D-80361
1-(2-Hydroxy-4-methoxyphenyl)-3-(3-hydroxy-4-methoxyphenyl)propane, *in* D-70336
1-(4-Hydroxy-2-methoxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)propane, *in* D-70336
1-(2-Hydroxy-4-methoxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)propene, *in* D-70336
1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, *in* C-80165
1-(6-Hydroxy-2-methoxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone, *in* M-70007
3-(4-Hydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* D-80366
1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxy-1-propenyl)-2-methoxyphenoxy]-1,3-propanediol, H-80193
2-(4-Hydroxy-2-methoxyphenyl)-6-methoxybenzofuran, *in* D-80363
8-(4-Hydroxy-3-methoxyphenyl)-3-methoxy-6,7-dimethyl-2-naphthol, *see* D-80025
2-(2-Hydroxy-4-methoxyphenyl)-6-methoxy-3-methylbenzofuran, H-70156
2-(2-Hydroxy-4-methoxyphenyl)-3-methoxy-5-(3-methyl-2-butenyl)-6-benzofuranol, *see* A-80057
2-(2-Hydroxy-4-methoxyphenyl)-7-methoxy-5-(1-propenyl)benzofuran, *in* H-60214
2-(2-Hydroxy-4-methoxyphenyl)-5,6-methylenedioxybenzofuran, *in* D-80355
1-(6-Hydroxy-2-methoxyphenyl)-9-(3,4-methylenedioxyphenyl)-1-nonanone, *in* M-70007
2-(2-Hydroxy-4-methoxyphenyl)-3-methyl-5,6-methylenedioxybenzofuran, H-70157
3-(4-Hydroxy-3-methoxyphenyl)-2-propenal, *see* C-80148
2-(2-Hydroxy-4-methoxyphenyl)-5-(1-propenyl)benzofuran, *in* H-60214
1-(2-Hydroxy-6-methoxyphenyl)-1-tetradecanone, *in* D-70338
1-(4-Hydroxy-3-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)-ethane, *in* D-80371
2-(3-Hydroxy-4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)ethanol, *see* C-70192
5-Hydroxy-7-methoxyphthalide, *in* D-60339
7-Hydroxy-5-methoxyphthalide, *in* D-60339
12-Hydroxy-13-methoxy-8,11,13-podocarpatriene-3,7-dione, *in* N-80028
1-Hydroxy-3-methoxy-7-primeverosyloxyxanthone, *in* T-80347
1-Hydroxy-7-methoxy-3-primeverosyloxyxanthone, *in* T-80347
7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone, *in* T-80347
3-Hydroxy-6-methoxyprimnatrienone, *in* P-80174
4-[2-Hydroxy-2-(2-methoxy-5-propenylphenyl)propyl]phenol, *see* H-80237
9-Hydroxy-3-methoxypterocarpan, *in* D-60373
6-Hydroxy-7-methoxyquinoxaline, *in* Q-60009
3-Hydroxy-5-methoxystilbene, *in* D-80384
6-(4-Hydroxy-3-methoxystyryl)-4-methoxy-2-pyrone, *in* H-70122
3-Hydroxy-4-methoxy-α-(3,4,5-trimethoxyphenyl)benzenemethanol, *see* C-70192
8-Hydroxy-3-methoxy-1,4,6-trimethyl-11-oxo-11*H*-dibenzo[*b*,*e*][1,4]dioxepin-7-carboxylic acid, *see* N-70081
2-Hydroxy-1-methoxyxanthone, *in* D-70353
2′-(Hydroxymethyl)acetophenone, H-70158
4′-(Hydroxymethyl)acetophenone, H-70159
8β-(2-Hydroxymethylacryloyloxy)hisutinolide 13-*O*-acetate, *in* H-80089
1-Hydroxy-4-(methylamino)anthraquinone, *in* A-60175
1-Hydroxy-7-methyl-9,10-anthracenedione, *see* H-60170
1-Hydroxy-7-methylanthraquinone, H-60170
2-(Hydroxymethyl)aziridine, H-80194
2-Hydroxy-4-methylbenzaldehyde, H-70160
2-(Hydroxymethyl)benzaldehyde, H-60171
3-Hydroxy-5-methylbenzaldehyde, H-80195
4-Hydroxy-2-methylbenzaldehyde, H-70161
α-Hydroxy-α-methylbenzeneacetaldehyde, *see* H-80240
5-Hydroxy-3-methyl-1,2-benzenedicarboxylic acid, H-70162
2-Hydroxymethyl-1,4-benzenediol, *see* D-70287
3-(Hydroxymethyl)-1,2-benzenediol, *see* D-80283
4-Hydroxymethyl-1,2-benzenediol, *see* D-80284
5-(Hydroxymethyl)-1,2,3-benzenetriol, H-80196
2-(Hydroxymethyl)-1,4-benzodioxan, H-60172
2-Hydroxy-4-methylbenzoic acid, H-70163
4-Hydroxy-2-methylbenzoic acid, H-70164
2-(Hydroxymethyl)benzonitrile, *see* I-70062
5-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one, H-60173
8-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one, H-70165

3-Hydroxymethylbicyclo[2.2.1]heptan-2-amine, *see* A-70093
3-Hydroxymethylbicyclo[2.2.1]hept-5-en-2-amine, *see* A-70094
Hydroxymethylbilane, H-70166
1-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]-2-(3,5-dihydroxyphenyl)ethylene, H-70167
5-[2-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]ethenyl]-1,3-benzenediol, *see* H-70167
2-(Hydroxymethyl)-1,4-butanediol, H-80197
4-(3-Hydroxy-3-methylbutanoyloxy)-3-(1,1-dimethyl-2-propenyl)-6-phenyl-2*H*-pyran-2-one, *in* D-70434
2-Hydroxy-3-methyl-2-butenenitrile, H-80198
4-Hydroxy-3-methylbut-2-enolide, *in* M-70103
5-Hydroxymethyl-2-butenolide, *see* H-60182
6-(3-Hydroxy-3-methyl-1-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, *see* S-70080
8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, *see* A-70269
8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxycoumarin, *see* A-70269
2-Hydroxy-5-(3-methyl-2-butenyl)-4-(1-methylethenyl)-2,4,6-cycloheptatrien-1-one, *see* P-80175
2-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-5,6-dimethoxy-3- benzofuranol, *see* L-80027
3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenoic acid, *see* D-80534
2-(Hydroxymethyl)-3-butyn-1-ol, *see* E-70054
2-Hydroxy-9-methylcarbazole, *in* H-60109
2-[(Hydroxymethyl)carbonyl]thiophene, *see* H-70103
5-Hydroxy-4-methylcoumarin, *see* H-60173
8-Hydroxy-4-methylcoumarin, *see* H-70165
2-Hydroxymethylcyclobutanecarboxylic acid lactone, *see* O-70053
2-Hydroxy-2-methylcyclobutanone, H-70168
4-Hydroxy-4-methyl-2,5-cyclohexadien-1-one, H-70169
5-(Hydroxymethyl)-1,2,3,4-cyclohexanetetrol, H-70170
1D-(1,2,4/3,5)-5-*C*-Hydroxymethyl-1,2,3,4-cyclohexanetetrol, *in* H-70170
1D-(1,2,4,5/3)-5-*C*-Hydroxymethyl-1,2,3,4-cyclohexanetetrol, *in* H-70170
1L-(1,2,4/3,5)-1-*C*-Hydroxymethyl-2,3,4,5-cyclohexanetetrol, *in* H-70170
1L-(1,3,5/2,4)-5-*C*-Hydroxymethyl-1,2,3,4-cyclohexanetetrol, *in* H-70170
2-Hydroxymethylcyclohexanol, *see* H-70120
5-Hydroxy-2-methylcyclohexanone, H-70171
5-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol, H-70172
2-Hydroxymethylcyclopentanecarboxylic acid lactone, *see* H-70054
▷ 2-Hydroxy-3-methyl-2-cyclopenten-1-one, H-60174
4-Hydroxy-2-methyl-2-cyclopenten-1-one, H-60175
5-(Hydroxymethyl)-2-cyclopenten-1-one, H-80199
2-Hydroxymethylcyclopropanecarboxylic acid lactone, *see* O-70055
3-Hydroxymethyldibenzo[*b,f*]thiepin, H-60176
8-Hydroxy-5-methyldihydrothiazolo[3,2-*a*]pyridinium-3-carboxylate, *see* C-70021
8-(Hydroxymethyl)-5,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* M-80198
8-Hydroxymethyl-5,7-dimethoxycoumarin, *in* M-80198
1-(Hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptane-2,3-diol, H-70173
2-Hydroxymethyl-1,1-dimethylcyclopropane, *see* D-70396
3-Hydroxymethyl-7,11-dimethyl-2,6,11-dodecatriene-1,5,10-triol, H-70174
2-Hydroxymethyl-1,1-dimethyloxirane, *see* D-70426
2-Hydroxymethyl-1,3-dioxolane, *see* D-70468
▷ *N*-Hydroxy-*N*-(15-methyl-3,10-dioxopentadecyl)seramide, *see* L-70033
16-Hydroxy-24-methyl-12,24-dioxo-25-scalaranal, H-80200
12α-Hydroxy-24-methyl-24,25-dioxo-14-scalaren-22-oic acid, *in* H-60191
(Hydroxymethyl)dodecahedrane, H-80201
2-(Hydroxymethylene)cyclohexanone, *see* O-80074
2-Hydroxy-4,5-methylenedioxybenzaldehyde, H-70175
2-Hydroxy-3,4-methylenedioxybenzoic acid, H-60177
2-Hydroxy-4,5-methylenedioxybenzoic acid, H-80202
3-Hydroxy-4,5-methylenedioxybenzoic acid, H-60178
4-Hydroxy-2,3-methylenedioxybenzoic acid, H-60179
6-Hydroxy-2,3-methylenedioxybenzoic acid, H-60180
5-Hydroxy-6,7-methylenedioxyflavone, *in* T-60322
7-Hydroxy-3′,4′-methylenedioxyisoflavone, H-80203
7-Hydroxy-3-(3,4-methylenedioxyphenyl)chromone, *see* H-80203
3-Hydroxy-8,9-methylenedioxypterocarpan, *see* M-70001
7-Hydroxy-4′,5′-methylenedioxypterocarpan (obsol.), *see* M-70001
3β-Hydroxy-24-methylene-8-lanosten-21-oic acid, *see* E-80001
Hydroxymethylenemalonic acid, *see* H-80204
Hydroxymethylenepropanedioic acid, H-80204
α-Hydroxymethylenepropiophenone, *see* B-80057
2-(1-Hydroxy-1-methylethyl)-5-benzofurancarboxaldehyde, *in* D-70214
4-Hydroxy-2-(1-methylethyl)-5-benzofurancarboxylic acid, *see* H-60164
1-[2-(1-Hydroxy-1-methylethyl)-5-benzofuranyl]ethanone, *see* A-70044
2-Hydroxy-2-(1-methylethyl)butanedioic acid, *see* H-60165
2-Hydroxy-3-(1-methylethyl)butanedioic acid, *see* H-60166
2-(1-Hydroxy-1-methylethyl)-5-methyltetrahydrofuran, *see* P-60160
6-Hydroxymethyleugenin, *see* H-60155
▷ 1-(Hydroxymethyl)fluorene, H-70176
▷ 5-Hydroxymethyl-2-furancarboxaldehyde, H-70177
5-Hydroxymethyl-2(5*H*)-furanone, H-60182
5-Hydroxy-4-methyl-2(5*H*)-furanone, *in* M-70103
▷ 5-Hydroxy-5-methyl-2(5*H*)-furanone, *see* O-70098
▷ 5-Hydroxymethylfurfural, *see* H-70177
5-(Hydroxymethyl)furfuryl alcohol, *see* B-60160
12-(Hydroxymethyl)-10-hentetraconten-4-ol, *see* N-70068
13-Hydroxymethyl-2,6,10,18,22,26,30-heptamethyl-14-methylene-10-hentriacontene, *see* T-70138
5-Hydroxy-4-methyl-3-heptanone, H-60183
6-Hydroxymethylherniarin, *in* H-70139
2-Hydroxy-2-methylhexanoic acid, H-60184
2-Hydroxy-3-methylhexanoic acid, H-60185
2-(6-Hydroxy-4-methyl-4-hexenylidene)-6,10-dimethyl-7-oxo-9-undecenal, H-60186
6-Hydroxymethylindole, *see* I-60032
7-Hydroxy-2-methylisoflavone, H-80205
7-Hydroxy-3-methylisoflavone, H-80206
6-Hydroxymethyllumazine, *see* H-80213
6-(Hydroxymethyl)-7-methoxy-2*H*-1-benzopyran-2-one, *in* H-70139
8-(Hydroxymethyl)-7-methoxy-2*H*-1-benzopyran-2-one, *see* M-80198
8-Hydroxymethyl-7-methoxycoumarin, *see* M-80198
1-[2-(Hydroxymethyl)-3-methoxyphenyl]-1,5-heptadiene-3,4-diol, H-70178
4-Hydroxymethyl-3-methyl-2-buten-1-olide, *see* H-60187
4*a*-Hydroxy-1-methyl-8-methylenegibbane-1,10-dicarboxylic acid 1,4*a*-lactone, *see* G-60018
2-(Hydroxymethyl)-5-(1-methylethyl)-1,4-benzenediol, *see* D-70309
3-Hydroxymethyl-2-methylfuran, H-80207
5-Hydroxymethyl-4-methyl-2(5*H*)-furanone, H-60187
6-(Hydroxymethyl)-10-methyl-2-(4-methyl-3-pentenyl)-2,6,10-dodecatriene-1,12-diol, H-70179
2-Hydroxymethyl-3-methyloxirane, *see* M-80128
3-(5-Hydroxymethyl-5-methyl-2-oxo-5*H*-furan-3-yl)-2-methylpropanoic acid, H-80208
11-Hydroxy-5-methyl-2-(1-methyl-1,3-pentadienyl)-8-[2,3,6-trideoxy-3-(dimethylamino)-β-D-*arabino*-hexopyranosyl]-10-[2,3,6-trideoxy-3-(dimethylamino)-3-*C*-methyl-α-L-*lyxo*-hexopyranosyl]-4*H*-anthra[1,2-*b*]pyran-4,7,12-trione, *see* R-70011
2-Hydroxymethyl-3-methylthiophene, *see* M-80176
2-Hydroxymethyl-4-methylthiophene, *see* M-80177
2-Hydroxymethyl-5-methylthiophene, *see* M-80178
3-(Hydroxymethyl)-2-naphthaldehyde, *see* H-60188
2-(Hydroxymethyl)naphthalene, *see* N-60004
3-(Hydroxymethyl)-2-naphthalenecarboxaldehyde, H-60188
5-Hydroxy-7-methyl-1,2-naphthalenedione, *see* H-60189
8-Hydroxy-3-methyl-1,2-naphthalenedione, *see* H-60190
5-Hydroxy-7-methyl-1,2-naphthoquinone, H-60189
8-Hydroxy-3-methyl-1,2-naphthoquinone, H-60190
2-Hydroxymethyl-3-nitroaniline, *see* A-80126
2-Hydroxymethyl-6-nitroaniline, *see* A-80125
3-Hydroxymethyl-2-nitroaniline, *see* A-80127
5-Hydroxymethyl-2-nitroaniline, *see* A-80128
2-Hydroxy-5-methyl-3-nitrobenzaldehyde, H-70180
3-(Hydroxymethyl)-7-oxabicyclo[4.1.0]hept-3-ene-2,5-dione, H-70181
2-Hydroxymethyloxetane, *see* O-80054
3-Hydroxymethyloxetane, *see* O-80055
4-Hydroxy-5-methyl-3-(8-oxofarnesyl)coumarin, *see* H-70183
12-Hydroxy-24-methyl-24-oxo-16-scalarene-22,25-dial, H-60191
3-Hydroxy-2-methylpentanoic acid, H-80209
3-Hydroxy-3-methylpentanoic acid, H-80210
5-Hydroxy-3-methylpentanoic acid, H-70182
5-Hydroxy-3-methyl-2-pentenoic acid, H-80211
2-Hydroxymethyl-4-penten-1-ol, *see* P-80180
5-Hydroxy-3-methyl-2-penten-4-olide, *see* H-60187
3-[2-[2-(5-Hydroxy-4-methyl-3-pentenyl)-2-methyl-2*H*-1-benzopyran-6-yl]ethyl]-1,2-benzenediol, *see* T-70008
9-Hydroxymethylphenanthrene, *see* P-80079
p-Hydroxymethylphenol, *see* H-80114
Hydroxymethylphenylacetylene, *see* P-60130
4-Hydroxy-α-methylphenylalanine, *see* A-60220
7-Hydroxy-2-methyl-3-phenyl-4*H*-1-benzopyran-4-one, *see* H-80205
7-Hydroxy-3-methyl-2-phenyl-4*H*-1-benzopyran-4-one, *see* H-80206

1-[2-(Hydroxymethyl)phenyl]ethanone, *see* H-70158
1-[4-(Hydroxymethyl)phenyl]ethanone, *see* H-70159
5-Hydroxy-3-methylphthalic acid, *see* H-70162
3-Hydroxy-3-methylphthalide, *see* A-80015
12-Hydroxy-13-methyl-8,11,13-podocarpatrien-7-one, *see* N-80027
2-Hydroxymethyl-1,3-propanediol, H-80212
6-(Hydroxymethyl)-2,4(1*H*,3*H*)pteridinedione, H-80213
3-Hydroxy-6-methylpyridazine, *in* M-70124
4-Hydroxy-6-methylpyridazine, *see* M-80151
4-Hydroxy-6-methyl-3-pyridinecarboxylic acid, *see* D-80224
3-Hydroxy-2-methyl-4(1*H*)-pyridinone, H-80214
p-Hydroxy-β-methylstyrene, *see* P-80179
5-Hydroxymethyl-2,2′:5,2″-terthiophene, *see* T-80011
6-(Hydroxymethyl)tetrahydro-2*H*-pyran-2-one, *in* D-60329
2-Hydroxymethyl-1-tetralol, *see* T-70064
7-Hydroxymethyl-2,6,10,14-tetramethyl-2,9*E*,13*E*-pentadecatrien-6-ol, *see* P-80075
2-Hydroxymethyl-5-(2-thienylethynyl)thiophene, *see* T-80180
4-Hydroxy-9-(methylthio)-2,4,8-decatrien-6-ynoic acid γ-lactone, *see* M-80172
2-(Hydroxymethyl)thiophenol, *see* M-80021
3-(Hydroxymethyl)thiophenol, *see* M-80022
4-(Hydroxymethyl)thiophenol, *see* M-80023
3-Hydroxymethyl-7,11,15-trimethyl-2,6,10-hexadecatriene-1,14,15-triol, H-80215
4-Hydroxy-5-methyl-3-(3,8,11-trimethyl-8-oxo-2,6,10-dodecatrienyl)-2*H*-1-benzopyran-2-one, H-70183
3-Hydroxy-5-methyl-2,4,6-trinitrobenzoic acid, H-60193
(2-Hydroxy-6-methyl-2,4,6-triphenyl-3-cyclohexen-1-yl)phenylmethanone, *see* D-60524
3-Hydroxy-2-methylvaleric acid, *see* H-80209
3-Hydroxy-3-methylvaleric acid, *see* H-80210
5-Hydroxy-3-methylvaleric acid, *see* H-70182
5-(Hydroxymethyl)-δ-valerolactone, *in* D-60329
Hydroxyminaline, *see* H-80249
3-Hydroxymugeneic acid, *in* M-60148
11β-Hydroxynanuzone, *in* E-80033
6-Hydroxy-1-naphthaldehyde, H-70184
6-Hydroxy-2-naphthaldehyde, H-70185
7-Hydroxy-2-naphthaldehyde, H-70186
1-Hydroxy-2-naphthaleneacrylic acid δ-lactone, *see* N-70011
6-Hydroxy-1-naphthalenecarboxaldehyde, *see* H-70184
6-Hydroxy-2-naphthalenecarboxaldehyde, *see* H-70185
7-Hydroxy-2-naphthalenecarboxaldehyde, *see* H-70186
4-Hydroxy-1,2-naphthalenedione, *see* H-60194
3-Hydroxynaphtho[*a*]cyclobutene, *see* D-60215
4-Hydroxy-1,2-naphthoquinone, H-60194
12-Hydroxynerolidol, *in* T-70283
13-Hydroxynerolidol, *in* T-70283
Hydroxyniranthin, H-70187
2-Hydroxy-5-nitro-1,3-benzenedicarboxylic acid, H-70188
3-Hydroxy-6-nitro-1,2-benzenedicarboxylic acid, H-70189
4-Hydroxy-3-nitro-1,2-benzenedicarboxylic acid, H-70190
4-Hydroxy-5-nitro-1,2-benzenedicarboxylic acid, H-70191
4-Hydroxy-5-nitro-1,3-benzenedicarboxylic acid, H-70192
2-Hydroxy-3-nitrobenzotrifluoride, *see* N-60050
2-Hydroxy-5-nitrobenzotrifluoride, *see* N-60053
3-Hydroxy-2-nitrobenzotrifluoride, *see* N-60047
3-Hydroxy-4-nitrobenzotrifluoride, *see* N-60049
4-Hydroxy-2-nitrobenzotrifluoride, *see* N-60051
▷ 4-Hydroxy-3-nitrobenzotrifluoride, *see* N-60048
2-Hydroxy-5-nitroisophthalic acid, *see* H-70188
4-Hydroxy-5-nitroisophthalic acid, *see* H-70192
2-Hydroxy-3-nitro-1,4-naphthalenedione, *see* H-60195
2-Hydroxy-3-nitro-1,4-naphthoquinone, H-60195
3-Hydroxy-6-nitrophthalic acid, *see* H-70189
4-Hydroxy-3-nitrophthalic acid, *see* H-70190
4-Hydroxy-5-nitrophthalic acid, *see* H-70191
▷ 1-Hydroxy-2-nitropyrene, *see* N-80058
4-Hydroxy-3-nitropyridine, *see* N-70063
▷ *N*-Hydroxy-*N*-nitrosoaniline, *see* H-70208
4-Hydroxy-3-nitrosobenzaldehyde, H-60197
▷ *N*-Hydroxy-*N*-nitrosobenzenamine, *see* H-70208
4-Hydroxy-3-nitrosobenzoic acid, H-70193
6-Hydroxy-5-nitro-*m*-tolualdehyde, *see* H-70180
▷ 4-Hydroxynonanoic acid γ-lactone, *see* D-70245
9-Hydroxy-5-nonenoic acid, H-70194
3α-Hydroxynorambreinolide, *in* N-80075
ent-1β-Hydroxy-3-nor-15-beyerene-2,12-dione, H-80216
ent-10β-Hydroxy-20-nor-16-gibberellene-7,19-dioic acid 19,10-lactone, *see* G-60018
11-Hydroxy-20-nor-8,15-isopimaradien-7-one, H-80217
6β-Hydroxynorjuslimdiolone, *in* N-60061
15-Hydroxy-17-nor-8-labden-7-one, H-60198
3-Hydroxy-30-nor-12,18-oleanadien-29-oic acid, H-80218
3-Hydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, H-60199
3β-Hydroxy-28-noroleana-12,17-dien-16-one, *in* M-70011
18β-Hydroxy-28-nor-3,16-oleanenedione, *in* D-60363
3β-Hydroxy-28-norolean-12-en-16-one, *see* M-70011
3-Hydroxy-16-nor-7-pimaren-15-oic acid, H-80219
6-Hydroxy-7,9-octadecadiene-11,13,15,17-tetraynoic acid, H-70195
13-Hydroxy-9,11-octadecadienoic acid, H-70196
17-Hydroxyoctadecanoic acid, H-80220
3-Hydroxy-28,13-oleananolide, H-60200
3β-Hydroxy-18α-olean-12-ene-27,28-dioic acid, *see* C-70002
3-Hydroxy-12-oleanen-30-oic acid, H-80222
3-Hydroxy-12-oleanen-29,22-olide, H-70197
16-Hydroxy-18-oleanen-3-one, H-80223
3-Hydroxy-12-oleanen-1-one, H-80224
16β-Hydroxy-18-oleanen-3-one, *in* O-80033
Hydroxyoleanonic lactone, *in* H-70201
4-Hydroxy-10(15)-oplopen-3-one, H-80225
3-Hydroxyornithine, *see* D-70039
5-Hydroxy-7-oxabicyclo[4.1.0]hept-2-ene-3-carboxylic acid, *see* E-80030
3-Hydroxy-1,2,4-oxadiazolidin-5-one, *see* O-70060
17-Hydroxy-15,17-oxido-16-spongianone, H-60201
15-Hydroxy-3-oxoalloalantolactone, *in* A-80044
6-Hydroxy-3-oxo-8′-apo-ε-caroten-8′-oic acid, *see* C-60156
4-Hydroxy-α-oxobenzenepropanoic acid, *see* H-80238
2-(7-Hydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-5-methoxy-2,5-cyclohexadiene-1,4-dione, *see* B-70175
10-Hydroxy-3-oxoborneol, *in* H-70173
3-Hydroxy-2-oxobutanoic acid, H-80226
4-Hydroxy-2-oxobutanoic acid, H-80227
6-(2-Hydroxy-3-oxobutyl)-7-methoxy-2*H*-1-benzopyran-2-one, *see* F-70046
2-Hydroxy-12-oxo-4,11(13)-cadinadien-15-oic acid, H-80228
7-Hydroxy-6-oxocarnosic acid, *see* T-60337
ent-4α-Hydroxy-3-oxo-13-cleroden-15,16-olide, *in* D-80303
2-[[[(1-Hydroxy-6-oxo-2-cyclohexen-1-yl)carbonyl]oxy]methyl]phenyl β-D-glucopyranoside, *see* S-70002
4-Hydroxy-1-oxo-2,11(13)-eudesmadien-12,8-olide, H-70198
8-Hydroxy-3-oxo-1,4,11(13)-eudesmatrien-12-oic acid, H-70199
9-Hydroxy-3-oxo-1,4(15),11(13)-eudesmatrien-12,6-olide, H-60202
6-Hydroxy-5-oxo-7,15-fusicoccadien-15-al, H-60203
8α-Hydroxy-2-oxo-4,10(14)-germacradien-12,6α-olide, *in* D-80319
5β-Hydroxy-2-oxo-1(10),3,11(13)-guaiatrien-12-oic acid, *see* H-70235
9β-Hydroxy-3-oxo-10(14)-guaien-12,6α-olide, *in* D-70305
ent-3β-Hydroxy-2-oxo-7,13-labdadien-15-al, *in* D-80328
3-Hydroxy-8-oxo-2(9),6-lactaradien-5,13-olide, H-80229
7-Hydroxy-3-oxo-8,24-lanostadien-26-al, H-70200
11-Hydroxy-3-oxo-13-nor-7(11)-eudesmen-12,6-olide, H-60204
12-Hydroxy-3-oxo-28,13-oleananolide, H-70201
3-Hydroxy-23-oxo-12-oleanen-28-oic acid, H-80230
19α-Hydroxy-3-oxo-12-oleanen-28-oic acid, *in* D-70327
26-Hydroxy-28-oxooligomycin *A*, *see* O-70039
2-Hydroxy-5-oxo-β-pinene, *see* H-80247
3-Hydroxy-1-oxo-1*H*-pyrazolo[1,2-*a*]pyrazol-4-ium hydroxide inner salt, *see* O-60092
22-Hydroxy-3-oxo-12-ursen-30-oic acid, H-70202
19α-Hydroxy-3-oxo-12-ursen-28-oic acid, *in* D-70350
8-Hydroxy-9-oxo-9*H*-xanthene-1-carboxylic acid, *see* H-80266
11-Hydroxypalmitic acid, *see* H-80172
10-Hydroxypalmitone, *see* H-80170
2-Hydroxy-6-(8,11-pentadecadienyl)benzoic acid, H-60205
2-Hydroxy-6-(8,11,14-pentadecatrienyl)benzoic acid, *in* H-60205
2-Hydroxy-6-(10-pentadecenyl)benzoic acid, *in* H-60205
2-Hydroxy-6-(8-pentadecenyl)benzoic acid, *in* H-60205
2-Hydroxy-6-(2,4-pentadiynyl)benzoic acid, H-80231
4′-Hydroxy-3,3′,5,6,7-pentamethoxyflavone, *in* H-80067
4′-Hydroxy-3′,5,5′,6,7-pentamethoxyflavone, *in* H-70081
5-Hydroxy-3,3′,4′,6,7-pentamethoxyflavone, *in* H-80067
6-Hydroxy-2′,3,5,5′,7-pentamethoxyflavone, *in* H-60064
7-Hydroxy-3,3′,4′,5,6-pentamethoxyflavone, *in* H-80067
Hydroxypentamethylbenzene, *see* P-60058
10-Hydroxy-1,2,5,7,9-pentamethyl-3,11,12-trioxatricyclo[5.3.1.1^{2,6}]dodecan-4-one, *see* B-70174
20ξ-Hydroxy-3,7,11,15,23-pentaoxo-8-lanosten-26-oic acid, *in* D-60379
▷ 4-Hydroxy-2-pentenoic acid γ-lactone, *see* M-60083
▷ 4-Hydroxy-3-pentenoic acid γ-lactone, *see* M-70081

4-Hydroxy-3-penten-2-one, *in* P-60059
3-Hydroxy-2-(2-pentenyl)cyclopentaneacetic acid, *see* C-50302
11-Hydroxy-1-[3-(2-pentenyl)oxiranyl]-9-undecenoic acid, *see* H-70127
4-Hydroxy-6-pentyl-*o*-anisic acid 2,4-dimethoxy-6-pentylbenzoate, *see* P-80158
1-Hydroxy-6-pentyl-5,15-dioxabicyclo[10.2.1]pentadecane-4,13-dione, *see* G-60025
5-Hydroxy-13(3-pentyloxiranyl)-6,8,10,12-tridecatetraenoic acid, *see* E-70016
13-[3-(5-Hydroxypentyl)oxiranyl]-5,8,11-tridecatrienoic acid, *see* E-70018
4-Hydroxy-2-pentyne, *see* P-70041
5-Hydroxy-4-phenanthrenecarboxylic acid, H-80232
2-Hydroxy-3*H*-phenoxazin-3-one, H-60206
(2-Hydroxyphenoxy)acetic acid, H-70203
(3-Hydroxyphenoxy)acetic acid, H-70204
(4-Hydroxyphenoxy)acetic acid, H-70205
2-Hydroxy-2-phenylacetaldehyde, H-60210
2-Hydroxyphenylacetaldehyde, H-60207
3-Hydroxyphenylacetaldehyde, H-60208
4-Hydroxyphenylacetaldehyde, H-60209
4-Hydroxyphenylacetaldoxime, *in* H-60209
N-Hydroxyphenylacetamide, *see* P-70059
p-Hydroxyphenylacetone, *see* H-80241
9-Hydroxy-10-phenylanthracene, *see* P-80089
2-Hydroxy-*N*-phenylbenzamide, *in* H-70108
2-(4-Hydroxyphenyl)benzoic acid, *see* H-70111
3-(3-Hydroxyphenyl)-1*H*-2-benzopyran-1-one, H-70207
6-Hydroxy-2-phenyl-4*H*-1-benzopyran-4-one, *see* H-70130
7-Hydroxy-2-phenyl-4*H*-1-benzopyran-4-one, *see* H-70131
4-Hydroxy-1-phenyl-2-butyn-1-one, H-80233
6-Hydroxy-2-phenylchromone, *see* H-70130
7-Hydroxy-2-phenylchromone, *see* H-70131
▷ 1-Hydroxy-2-phenyldiazene 2-oxide, H-70208
3-(4-Hydroxyphenyl)-1-(2,4-dihydroxy-6-methoxyphenyl)-1-propanone, *in* H-80246
5-[2-(3-Hydroxyphenyl)ethenyl]-1,2,4-benzenetriol, *see* H-70215
6-[2-(4-Hydroxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one, *see* H-70122
2-[2-(4-Hydroxyphenyl)ethenyl]phenol, *see* D-80379
3-[2-(4-Hydroxyphenyl)ethenyl]phenol, *see* D-80383
4-[2-(3-Hydroxyphenyl)ethyl]-1,2-benzenediol, *see* T-60316
5-[2-[(3-Hydroxyphenyl)ethyl]]-1,2,3-benzenetriol, *see* T-60102
4-[2-(3-Hydroxyphenyl)ethyl]-2,6-dimethoxyphenol, *in* T-60102
▷ (4-Hydroxyphenyl)ethylene, H-70209
4-Hydroxyphenyl β-D-glucopyranoside, *see* A-70248
▷ 5-Hydroxy-7-phenyl-2,6-heptadienoic acid lactone, *see* G-60031
7-(3-Hydroxyphenyl)-2-heptene-4,6-diyn-1-ol, H-80234
6-Hydroxy-1-phenyl-2,4-hexadiyn-1-one, H-80235
3-(4-Hydroxyphenyl)-1-(2-hydroxy-4,6-dimethoxyphenyl)-2-propen-1-one, *in* H-80246
5-(4-Hydroxyphenyl)-2-(4-hydroxy-3-methoxyphenyl)-3,4-dimethyltetrahydrofuran, *in* T-60061
1-(2-Hydroxyphenyl)-2-(4-hydroxyphenyl)ethylene, *see* D-80379
1-(3-Hydroxyphenyl)-2-(4-hydroxyphenyl)ethylene, *see* D-80383
2-(4-Hydroxyphenyl)-5-(2-Hydroxypropyl)-3-methylbenzofuran, H-80236
2-(4-Hydroxyphenyl)-5-(3-hydroxypropyl)-3-methylbenzofuran, *see* O-60040
3-(3-Hydroxyphenyl)isocoumarin, *see* H-70207
3-Hydroxy-4-phenyl-5(2*H*)-isoxazolone, *see* D-70337
5-Hydroxy-4-phenyl-3(2*H*)-isoxazolone, *see* D-70337
2-(4-Hydroxyphenyl)-7-methoxy-3-methyl-5-propenylbenzofuran, *in* K-60001
3-Hydroxy-2-(phenylmethoxy)propanal, *see* B-80058
2-(4-Hydroxyphenyl)-7-methoxy-5-(1-propenyl)benzofuran, *in* H-60214
2-(4-Hydroxyphenyl)-7-methoxy-5-(1-propenyl)-3-benzofurancarboxaldehyde, H-60212
1-(4-Hydroxyphenyl)-2-(2-methoxy-4-propenylphenoxy)-1-propanol, *in* H-60215
1-(4-Hydroxyphenyl)-2-(2-methoxy-5-propenylphenyl)-2-propanol, H-80237
2-(4-Hydroxyphenyl)-3-methyl-5-benzofuranpropanol, *see* O-60040
2-(4-Hydroxyphenyl)-3-methyl-5-(2-oxopropyl)benzofuran, *in* H-80236
2-(4-Hydroxyphenyl)-3-methyl-5-(1-propenyl)benzofuran, *see* E-60075
3-(4-Hydroxyphenyl)-2-oxopropanoic acid, H-80238
1-(2-Hydroxyphenyl)-2-phenylethane, *see* P-70071
1-(3-Hydroxyphenyl)-2-phenylethane, *see* P-70072
1-(4-Hydroxyphenyl)-2-phenylethane, *see* P-70073
1-(2-Hydroxyphenyl)-3-phenyl-1,3-propanedione, H-80239
2-Hydroxy-2-phenylpropanal, H-80240
1-(4-Hydroxyphenyl)-2-propanone, H-80241
3-(4-Hydroxyphenyl)-2-propenal, H-60213
1-(4-Hydroxyphenyl)-2-propene, *see* P-80179
▷ 3-(4-Hydroxyphenyl)-2-propenoic acid, H-80242
2-(4-Hydroxyphenyl)-5-(1-propenyl)benzofuran, H-60214
1-(4-Hydroxyphenyl)-2-(4-propenylphenoxy)-1-propanol, H-60215
2-Hydroxy-2-phenylpropiophenone, *see* H-70123
2-Hydroxy-3-phenylpropiophenone, *see* H-70124
1-(4-Hydroxyphenyl)pyrrole, H-60216
2-(2-Hydroxyphenyl)pyrrole, H-60217
p-Hydroxyphenylpyruvic acid, *see* H-80238
8-Hydroxy-7-phenylquinoline, H-60218
4-Hydroxy-2-phenylquinoline, *in* P-60132
2-Hydroxy-4-phenylquinoline, *see* P-60131
5-Hydroxy-2-(phenylthio)-1,4-naphthalenedione, *see* H-70213
5-Hydroxy-3-(phenylthio)-1,4-naphthalenedione, *see* H-70214
5-Hydroxy-2-(phenylthio)-1,4-naphthoquinone, H-70213
5-Hydroxy-3-(phenylthio)-1,4-naphthoquinone, H-70214
1-(3-Hydroxyphenyl)-2-(2,4,5-trihydroxyphenyl)ethylene, H-70215
1-(4-Hydroxyphenyl)-3-(2,4,6-trihydroxyphenyl)-1-propanone, H-80243
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone, H-80244
3-(4-Hydroxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, H-80245
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one, H-80246
ent-12β-Hydroxy-8(14),15-pimaradien-3-one, *in* P-80146
ent-3β-Hydroxy-8(14),15-pimaradien-12-one, *in* P-80146
2-Hydroxy-1(10)-pinen-5-one, H-80247
1-Hydroxypinoresinol, H-60221
9-Hydroxypinoresinol, H-70216
2-Hydroxypiperonylic acid, *see* H-60177
6-Hydroxypiperonylic acid, *see* H-80202
4-Hydroxy-2-prenylcinnamic acid, *see* D-80534
6-Hydroxyprimnatrienone, *in* P-80174
Hydroxyproline leucine anhydride, *see* C-60213
Hydroxyprolylproline anhydride, *see* O-60017
3-Hydroxy-2-propenoic acid, *in* O-60090
4-(3-Hydroxy-1-propenyl)-2,6-dimethoxyphenol, *see* S-70046
5-(2-Hydroxypropyl)-7-methoxy-2-(3,4-methylenedioxyphenyl)benzofuran, *see* E-70001
6-(1-Hydroxypropyl)-1-methyllumazine, *see* L-70029
3-Hydroxy-5-(1-propynyl)-2-thienyl methyl ketone, *see* A-80024
1-[3-Hydroxy-5-(1-propynyl)-2-thiophenyl]ethanone, *see* A-80024
5-Hydroxypseudobaptigenin, *in* T-80109
5′-Hydroxypsorospermin, *in* P-70132
2-Hydroxypterocarpin, *in* T-80117
4-Hydroxypterocarpin, *in* T-80119
11-Hydroxyptilosarcenone, *in* P-60193
6α-Hydroxypulchellin, *in* P-80189
6β-Hydroxypulchellin 2-*O*-acetate, *in* P-80189
6α-Hydroxypulchellin 4-*O*-angelate, *in* P-80189
6β-Hydroxypulchellin 2-*O*-isovalerate, *in* P-80189
3-Hydroxy-2-pyridinamine, *see* A-60200
3-Hydroxy-4-pyridinamine, *see* A-60202
5-Hydroxy-2-pyridinamine, *see* A-60201
5-Hydroxy-3-pyridinamine, *see* A-60203
▷ 1-Hydroxy-2(1*H*)-pyridinethione, H-70217
3-Hydroxy-2(1*H*)-pyridinethione, H-60222
3-Hydroxy-2(1*H*)-pyridinone, H-60223
3-Hydroxy-4(1*H*)-pyridinone, H-60227
4-Hydroxy-2(1*H*)-pyridinone, H-60224
5-Hydroxy-2(1*H*)-pyridinone, H-60225
6-Hydroxy-2(1*H*)-pyridinone, H-60226
2-Hydroxy-4(1*H*)-pyridinone, *in* H-60224
2-Hydroxy-1-(2-pyridinyl)ethanone, *see* H-70101
2-Hydroxy-1-(3-pyridinyl)ethanone, *see* H-70102
3-Hydroxypyrrole, *see* D-70262
3-Hydroxy-1*H*-pyrrole-2-carboxylic acid, H-80248
4-Hydroxy-1*H*-pyrrole-2-carboxylic acid, H-80249
4-Hydroxy-1*H*-pyrrole-3-carboxylic acid, H-80250
3-Hydroxy-1*H*-pyrrole-2,4-dicarboxylic acid, H-80251
3-Hydroxy-1*H*-pyrrole-2,5-dicarboxylic acid, H-80252
3-Hydroxypyrrolidine, *see* P-70187
3-Hydroxypyrrolidine-2-acetic acid lactone, *see* H-80059
3-Hydroxyquinaldic acid, *see* H-60228
2-Hydroxy-4-quinazolinethione, *see* D-60295
N-Hydroxy-4-quinolinamine, H-80253
3-Hydroxy-2-quinolinecarboxylic acid, H-60228
8-Hydroxy-9-β-D-ribofuranosylguanine, *see* D-70238
▷ 8′-Hydroxyrotenone, *see* A-80152
2β-Hydroxyroyleanone, *in* R-60015
7-Hydroxyroyleanone, *see* D-80265
2α-Hydroxysalvicanaric acid, *in* S-70004
8α-Hydroxysambucoin, *in* S-70007
8β-Hydroxysambucoin, *in* S-70007
8-Hydroxy-15-sandaracopimarene, *see* H-60163
6α-Hydroxysandaracopimaric acid, *in* S-80008
7α-Hydroxysandaracopimaric acid, *in* S-80008
12β-Hydroxysandaracopimaric acid, *in* S-80008
3β-Hydroxysandaracopimaric acid, *in* S-80008
9α-Hydroxysantamarine, *in* S-60007
4-Hydroxysapriparaquinone, H-80254
ent-15-Hydroxy-8,9-seco-13-labdene-8,9-dione, H-70218

1*R*-Hydroxy-3,4-seco-4(23),20(29)-lupadiene-3,28-dioic acid 3,11α-lactone, *see* C-70038
3-Hydroxyselenetane, *see* S-80022
9-Hydroxysemperoside, *in* S-60021
6-Hydroxyskimmin, *in* D-84287
15-Hydroxysolavetivone, *in* S-70051
6-Hydroxy-3-spirostanone, H-70219
19-Hydroxy-13(16),14-spongiadien-3-one, H-70220
2-Hydroxy-1,15-stachadien-3-one, *see* H-80115
3-Hydroxy-15-stachen-2-one, *see* H-80116
17-Hydroxystearic acid, *see* H-80220
13-Hydroxysterpuric acid, *in* S-60053
▷ 4-Hydroxystyrene, *see* H-70209
α-Hydroxystyrene, *see* P-60092
6-(4-Hydroxystyryl)-4-methoxy-2-pyrone, *see* H-70122
4-Hydroxystyryl 2,3,4-trihydroxyphenyl ketone, *see* H-80245
4-Hydroxystyryl 2,4,6-trihydroxyphenyl ketone, *see* H-80246
Hydroxysuccinic anhydride, *see* D-80211
2α-Hydroxysugiol, *in* D-70281
6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid, H-80255
6-Hydroxysumatrol, *in* S-80051
1-Hydroxysyringaresinol, *in* H-60221
3-Hydroxytaraxastan-28,20-olide, H-70221
3-Hydroxy-14-taraxeren-28-oic acid, H-80256
2α-Hydroxytaxodione, *in* D-70282
2α-Hydroxytaxodone, *in* D-70282
11-Hydroxytephrosin, *in* T-80009
Hydroxyterephthalic acid, *see* H-70105
1-(2′-Hydroxy[1,1′:3′,1″-terphenyl]-5′-yl)-2,4,6-triphenylpyridinium hydroxide inner salt,9CI, *see* T-80362
6-Hydroxy-2,4,8-tetradecatrienoic acid, H-70222
3-(14-Hydroxy-2,5,8-tetradecatrienyl)oxiranebutanoic acid, *see* E-70017
12-Hydroxy-13-tetradecenoic acid, H-60229
14-Hydroxy-12-tetradecenoic acid, H-60230
9β-Hydroxy-4β,11β,13,15-tetrahydrodehydrozaluzanin *C*, *in* D-70305
3-Hydroxytetrahydrofuranone, *see* D-60242
4-Hydroxy-1,2,3,4-tetrahydroisoquinoline, *see* T-60066
5-Hydroxy-1,2,3,4-tetrahydroisoquinoline, *see* T-80065
7-Hydroxy-1,2,3,4-tetrahydroisoquinoline, *see* T-80066
9β-Hydroxy-4β,11α,13,15-tetrahydrozaluzanin *C*, *in* D-70305
9β-Hydroxy-4β,11β,13,15-tetrahydrozaluzanin *C*, *in* D-70305
5-Hydroxy-2′,3,7,8-tetramethoxyflavone, *in* P-70029
5-Hydroxy-2′,4′,7,8-tetramethoxyflavone, *in* P-80034
5-Hydroxy-3,4′,6,7-tetramethoxyflavone, *in* P-80035
5-Hydroxy-2′,4′,5′,7-tetramethoxyisoflavone, *in* P-80041
7-Hydroxy-2′,4′,5′,6-tetramethoxyisoflavone, *in* P-80042
7-Hydroxy-5,5′,6,8-tetramethoxy-3′,4′-methylenedioxyflavone, *in* H-80029
8-Hydroxy-3,4,9,10-tetramethoxypterocarpan, *in* P-80055
12-Hydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenoic acid, H-70223
16-Hydroxy-2,6,10,14-tetramethyl-2,6,10,14-hexadecatetraenoic acid, H-70224
2-(5-Hydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-6-methyl-1,2-benzenediol, H-70225
ent-7β-Hydroxy-13,14,15,16-tetranor-3-cleroden-12-oic acid 18,19-lactone, H-70226
ent-12-Hydroxy-13,14,15,16-tetranor-1(10)-halimen-18-oic acid, H-60231
15α-Hydroxy-3,7,11,23-tetraoxo-8,20*E*-lanostadien-26-oic acid, *in* D-80390
3β-Hydroxy-7,11,15,23-tetraoxo-8,20*E*-lanostadien-26-oic acid, *in* D-80390
7β-Hydroxy-3,11,15,23-tetraoxo-8,20(22)-lanostadien-26-oic acid, *in* T-70254
12α-Hydroxy-3,7,11,15-tetraoxo-25,26,27-trisnor-8-lanosten-24-oic acid, *in* L-60037
6-Hydroxy-1,2,4,5-tetrazin-3(2*H*)-one, *see* D-70268
2-Hydroxythiochromone, *see* H-70110
4-Hydroxythiocoumarin, *see* H-70110
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5-Hydroxy-4′,6,7-trimethoxyisoflavone, *in* T-80112
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8-Hydroxytriptiliocoumarin, *in* T-80363
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5-Methoxy-2,2-dimethyl-6-(2-methyl-1-oxo-2-butenyl)-10-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-8-one, M-80042
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7-Methoxyflavone, *in* H-70131
8-Methoxyflavone, *in* H-70132
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3-Methoxy-2(5*H*)-furanone, M-80043
4-Methoxy-2(5*H*)-furanone, *in* F-80087
▷ 9-Methoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, *see* X-60001
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▷ 8-Methoxy-4′,5′:6,7-furocoumarin, *see* X-60001
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2-(9-Methoxygeranylgeranyl)-6-methyl-1,4-benzoquinone, *in* S-60010
3′-Methoxyglabridin, *in* G-70016
8-Methoxyguanosine, *in* D-70238
1-Methoxy-1-hexene, M-70046
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2-Methoxyhomopterocarpin, *in* T-80335
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7-Methoxyindeno[1,2,3-*cd*]pyrene, *in* I-60025
8-Methoxyindeno[1,2,3-*cd*]pyrene, *in* I-60026
6-Methoxyindole, *in* H-60158
5-Methoxy-1*H*-indol-6-ol, *in* D-70307
6-Methoxy-1*H*-indol-5-ol, *in* D-70307
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3-Methoxy-1*H*-isoindole, *in* P-70100
6-Methoxyisoquinoline, *in* H-80178
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3′-Methoxyisosativanone, *in* T-80099
7α-Methoxy-8-labdene-3β,15-diol, *in* L-70013
α-Methoxylidene-γ-butyrolactone, *see* D-70222
4-Methoxymaackiain, *in* T-80119
6β-Methoxymaackiain, *see* S-60038
2-Methoxymedicarpin, *in* T-80335
4-Methoxymedicarpin, *in* T-80336
N-Methoxymethanamine, *see* D-70418
6-Methoxy-3-(6-methoxy-1,3-benzodioxol-5-yl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4*b*′]dipyran-4-one, *see* I-80001
5-Methoxy-2-(6-methoxy-3-methyl-2-benzofuranyl)phenol, *see* H-70156
6-Methoxy-2-[2-(4-methoxyphenyl)ethyl]-4*H*-1-benzopyran-4-one, M-60039
6-Methoxy-2-[2-(4-methoxyphenyl)ethyl]chromone, *see* M-60039
2-Methoxy-6-[2-methoxy-4-(2-propenyl)phenoxy]-4-(2-propenyl)phenol, *see* D-80024
2-Methoxy-4-methylbenzaldehyde, *in* H-70160
3-Methoxy-5-methylbenzaldehyde, *in* H-80195
4-Methoxy-2-methylbenzaldehyde, *in* H-70161
3-Methoxy-6-methyl-1,2,4-benzenetriol, *in* M-80050
5-Methoxy-3-methyl-1,2,4-benzenetriol, *in* M-80048
6-Methoxy-3-methyl-1,2,4-benzenetriol, *in* M-80049
6-Methoxy-5-methyl-1,2,4-benzenetriol, *in* M-80049
2-Methoxy-4-methylbenzoic acid, *in* H-70163
4-Methoxy-2-methylbenzoic acid, *in* H-70164
8-Methoxy-4-methyl-2*H*-1-benzopyran-2-one, *in* H-70165
9-Methoxy-10-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,6-(11*aH*)-diol, *see* C-80156
6-Methoxy-7-[(3-methyl-2-butenyl)oxy]coumorin, *in* H-80189
4-Methoxy-3-(3-methyl-2-butenyl)-5-phenyl-2(5*H*)-furanone, M-70047
8-Methoxy-*N*-methylchlorotetracycline, *in* M-70045
5-Methoxy-4-methylcoumarin, *in* H-60173
8-Methoxy-4-methylcoumarin, *in* H-70165
2-Methoxy-3-methyl-2-cyclopenten-1-one, *in* H-60174
2-(Methoxymethylene)cyclohexanone, *in* O-80074
2-Methoxy-4,5-methylenedioxybenzaldehyde, *in* H-70175
2-Methoxy-3,4-methylenedioxybenzoic acid, *in* H-60177
3-Methoxy-4,5-methylenedioxybenzoic acid, *in* H-60178
4-Methoxy-2,3-methylenedioxybenzoic acid, *in* H-60179
6-Methoxy-2,3-methylenedioxybenzoic acid, *in* H-60180
6-Methoxy-3,4-methylenedioxybenzoic acid, *in* H-80202
3′-Methoxy-3,4-methylenedioxybibenzyl, *in* T-60316
3-Methoxy-4,5-methylenedioxycinnamaldehyde, *see* M-70048
5-Methoxy-6,7-methylenedioxyflavone, *in* T-60322
7-Methoxy-3′,4′-methylenedioxyisoflavone, *in* H-80203
6-(2-Methoxy-4,5-methylenedioxyphenyl)furocoumarin, *see* P-80003
3-(2-Methoxy-4,5-methylenedioxyphenyl)propenal, M-70048
4-Methoxy-6-(3,4-methylenedioxystyryl)-α-pyrone, *in* M-80086
5-Methoxy-2-(7-methylfuro[2,3-*f*]-1,3-benzodioxol-6-yl)phenol, *see* H-70157
4-Methoxy-7-methyl-5*H*-furo[2,3-*g*][2]benzopyran-5-one, *see* C-70198
6-Methoxy-5-methyl-1-hexene, *in* M-80104
2-Methoxy-4-methyl-4*H*-imidazo[4,5-*b*]pyrazine, *in* I-60006
6-Methoxy-3-methyl-4,5-isobenzofurandione, *see* A-60070
7-Methoxy-2-methylisoflavone, *in* H-80205
5-Methoxy-7-methyl-1,2-naphthoquinone, *in* H-60189
8-Methoxy-3-methyl-1,2-naphthoquinone, *in* H-60190
3-Methoxy-4,5-methylnedioxybenzonitrile, *in* H-60178
5-Methoxy-2-methyl-3-nitroaniline, *in* A-60222
3-Methoxy-2-methyl-6-nitrophenol, *in* M-70097
5-Methoxy-2-methyl-3-nonaprenyl-1,4-benzoquinone, *in* M-80046
5-Methoxy-2-methyl-3-octaprenyl-1,4-benzoquinone, *in* M-80046
3-Methoxy-4-methyl-1,2,4-oxadiazolidin-5(4*H*)-one, *in* O-70060
4-Methoxy-6-methyl-5-(1-oxo-2-butenyl)2-*H*-pyran-2-one, *see* P-80203
4-(Methoxymethyl)phenol, *in* H-80114
5-Methoxy-2-methyl-3-polyprenyl-1,4-benzoquinone, M-80046
3-Methoxy-6-methylpyridazine, *in* M-70124
2-Methoxy-1-methyl-4(1*H*)-pyridinone, *in* H-60224
3-Methoxy-1-methyl-4(1*H*)-pyridinone, *in* H-60227
3-Methoxy-2-methyl-4(1*H*)-pyridinone, *in* H-80214
4-Methoxy-1-methyl-2(1*H*)-pyridinone, *in* H-60224
Methoxymethyl salicylate, *in* H-70108
2-(5-Methoxy-5-methyltetrahydro-2-furanyl)-6,10-dimethyl-5,9-undecadien-2-ol, M-80047
4-Methoxy-5-methyl-6-(7,9,11-trimethyl-1,3,5,7,9,11-tridecahexaenyl)-2*H*-pyran-2-one, *see* C-60149
1-Methoxy-3-myodesertene, *in* M-80203
6-Methoxy-1-naphthaldehyde, *in* H-70184
6-Methoxy-2-naphthaldehyde, *in* H-70185
7-Methoxy-2-naphthaldehyde, *in* H-70186
4-Methoxy-1,2-naphthoquinone, *in* H-60194
3-Methoxy-6-nitro-1,2-benzenedicarboxylic acid, *in* H-70189
4-Methoxy-3-nitro-1,2-benzenedicarboxylic acid, *in* H-70190
4-Methoxy-5-nitro-1,2-benzenedicarboxylic acid, *in* H-70191
4-Methoxy-5-nitro-1,3-benzenedicarboxylic acid, *in* H-70192
2-Methoxy-5-nitrobenzotrifluoride, *in* N-60053
5-Methoxy-4-nitro-1-naphthol, *in* N-80054
6-Methoxy-1-nitro-2-naphthol, *in* N-80048
4-Methoxy-3-nitropyridine, *in* N-70063
1-Methoxy-2-nitro-4-(trifluoromethyl)benzene, *in* N-60048
1-Methoxy-3-nitro-5-(trifluoromethyl)benzene, *in* N-60052
1-Methoxy-4-nitro-2-(trifluoromethyl)benzene, *in* N-60053
4-Methoxy-1-nitro-2-(trifluoromethyl)benzene, *in* N-60054
1-Methoxy-2-nonyne, *in* N-80074
12-Methoxy-17-nor-8,11,13-abietatrien-15-one, *see* N-80031
11-Methoxynoryangonin, *in* H-70122
22α-Methoxy-13(18)-oleanen-3β,24-diol, *in* O-80040
3β-Methoxy-18-oleanene, *in* O-80041
8-Methoxyorobol, *in* P-80045
6-Methoxyorobol 7-methyl ether, *in* P-70032
5-Methoxy-3-(8,11,14)pentadecatrienyl)-1,2,4-benzenetriol, M-70049
Methoxypentamethylbenzene, *in* P-60058
4-Methoxy-3-penten-2-one, *in* P-60059
1-Methoxyphaseollidin, *in* P-80076
5-Methoxy-4-phenanthrenecarboxylic acid, *in* H-80232
4-Methoxy-2,5-phenanthrenediol, *in* P-60071
2-Methoxy-3*H*-phenoxazin-3-one, *in* H-60206
(2-Methoxyphenoxy)acetic acid, *in* H-70203
(3-Methoxyphenoxy)acetic acid, *in* H-70204
(4-Methoxyphenoxy)acetic acid, *in* H-70205
2-Methoxy-2-phenylacetaldehyde, *in* H-60210
(2-Methoxyphenyl)acetaldehyde, *in* H-60207
4-Methoxyphenylacetaldehyde, *in* H-60209
5-Methoxy-2-phenyl-7*H*-1-benzopyran-7-one, *see* N-70074
4-Methoxy-4-phenyl-1-butene, *in* P-70061
1-Methoxy-2-phenyldiazene 2-oxide, *in* H-70208
▷ 4-Methoxyphenyldiazomethane, *see* D-60064
1-Methoxy-2-phenyldiimine 2-oxide, *in* H-70208
3-(4-Methoxyphenyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, *see* C-80013
3-Methoxy-5-(2-phenylethenyl)phenol, *in* D-80384
5-[2-(3-Methoxyphenyl)ethyl]-1,3-benzodioxole, *in* T-60316

1-Methoxy-1-phenylethylene, *in* P-60092
(4-Methoxyphenyl)ethylene, *in* H-70209
3-Methoxy-5-(2-phenylethyl)phenol, *in* P-80100
6-Methoxy-2-phenyl-4*H*-furo[2,3-*h*]-1-benzopyran-4-one, *see* K-70003
6-Methoxy-2-phenyl-4*H*-furo[2,3-*h*]-1-benzopyran-4-one, *see* K-80002
1-Methoxy-2-(phenylmethoxy)benzene, *in* B-60072
1-Methoxy-3-(phenylmethoxy)benzene, *in* B-60073
1-Methoxy-4-(phenylmethoxy)benzene, *in* B-60074
2-Methoxy-1-phenylnaphthalene, *in* P-60115
2-Methoxy-5-phenylnaphthalene, *in* P-60118
7-Methoxy-1-phenylnaphthalene, *in* P-60119
3-Methoxy-4-phenyl-2-prenyl-2-butenolide, *see* M-70047
1-(4-Methoxyphenyl)-2-propanone, *in* H-80241
3-(4-Methoxyphenyl)-2-propenal, *in* H-60213
3-(4-Methoxyphenyl)-2-propenoic acid, *in* H-80242
1-(4-Methoxyphenyl)pyrrole, *in* H-60216
2-(2-Methoxyphenyl)pyrrole, *in* H-60217
2-Methoxy-4-phenylquinoline, *in* P-60131
4-Methoxy-2-phenylquinoline, *in* P-60132
5-Methoxy-2-(phenylthio)-1,4-naphthoquinone, *in* H-70213
5-Methoxy-3-(phenylthio)-1,4-naphthoquinone, *in* H-70214
3-(4-Methoxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, *in* H-80245
6-Methoxy-4-phenylumbelliferone, *see* I-60097
2-Methoxypiperonylic acid, *in* H-60177
5-Methoxypiperonylic acid, *in* H-60178
6-Methoxy-1,3-primnatrienedione, *in* P-80174
6-Methoxyprimnatrienone, *in* P-80174
▷ 1-Methoxy-2-propanol, *in* P-70118
▷ 1-Methoxy-4-(1-propenyl)benzene, *in* P-80179
4-[2-[2-Methoxy-5-(1-propenyl)phenyl]-2-propenyl]phenol, *see* H-60029
▷ 9-Methoxypsoralen, *see* X-60001
2-Methoxypterocarpin, *in* T-80117
4-Methoxypterocarpin, *in* T-80119
3-Methoxy-4(1*H*)-pyridinone, *in* H-60227
6-Methoxy-2(1*H*)-pyridinone, *in* H-60226
2-Methoxy-1-(2-pyridinyl)ethanone, *in* H-70101
1-[1-Methoxy-1-(2-pyridinyl)ethyl]isoquinoline, *in* I-60134
4-Methoxy-1*H*-pyrrole-3-carboxylic acid, *in* H-80250
4-Methoxy-2-pyrrolecarboxylic acid, *in* H-80249
2-Methoxy-1-pyrroline, *in* P-70188
7-Methoxyrosmanol, *in* R-70010
7α-Methoxyroyleanone, *in* D-80265
11′-Methoxysargaquinone, *in* S-60010
9′-Methoxysargaquinone, *in* S-60010
3α-Methoxy-14-serraten-21β-ol, *in* S-80027
3β-Methoxy-14-serraten-21α-ol, *in* S-80027
21β-Methoxy-14-serraten-3β-ol, *in* S-80027
3β-Methoxy-14-serraten-21β-ol, *in* S-80027
3′-Methoxy-3,4′5-stilbenetriol, *in* D-80361
5-Methoxy-3-stilbenol, *in* D-80384
α-Methoxystyrene, *in* P-60092
p-Methoxystyrene, *in* H-70209
2-Methoxysuccinic anhydride, *in* D-80211
2-Methoxy-1-(2-thienyl)ethanone, *in* H-70103
3-Methoxythiophene, *in* T-60212
4-Methoxy-2-(trifluoromethyl)benzaldehyde, *in* H-70228
4-Methoxy-3-(trifluoromethyl)benzaldehyde, *in* H-70229
3-Methoxy-6-[2-(3,4-5-trimethoxyphenyl)ethenyl]-1,2-benzenediol, *in* T-60344
3-Methoxy-6-[2-(3,4,5-trimethoxyphenyl)ethyl]1,2-benzenediol, *in* T-60344
5-Methoxy-1,2,3-trimethylbenzene, *in* T-60371
3-Methoxy-2,5,6-trimethylphenyl 3,5-diformyl-2,4-dihydroxy-6-methylbenzoate, *see* N-70032
10-Methoxy-1-undecyne, *in* U-80032
5-Methoxyvestitol, *in* T-80096
6-Methoxyvestitol, *in* T-80098
6-Methoxy-5-vinylbenzofuran, *in* H-70231
3-Methoxy-1-vinylcyclopentene, *in* V-80008
11-Methoxyyangonin, *in* H-70122
Methyl 3-formylcrotonate, *in* M-70103
Methyl 8α-acetoxy-3α-hydroxy-13,14,15,16-tetranorlabdan-12-oate, *in* D-80387
▷ Methyl acrylate, *in* P-70121
α-Methylacrylophenone, *see* M-80146
8β-(2-Methylacryloxyloxy)hirsutinolide, *in* H-80089
8β-(2-Methylacryloyloxy)hirsutinolide 13-*O*-acetate, *in* H-80089
8β-(2-Methylacryloyloxy)-15-hydroxyhisutinolide 13-acetate, *in* H-80089
1-Methyladamantanone, M-60040
5-Methyladamantanone, M-60041
7-Methyladenine, *see* A-60226
2-Methyladipaldehyde, *see* M-80096
▷ β-Methylaesculetin, *see* H-80189
O-Methylalloptaeroxylin, *in* A-60075
Methyl altamisate, *in* A-70084
▷ 4-(Methylamino)cycloheptanone, *see* P-60151
8-(Methylamino)guanosine, *in* A-70150
(Methylamino)methanesulfonic acid, *in* A-60215
Methyl 3-amino-2-formyl-2-propenoate, *in* A-80134
2-(Methylamino)-4(1*H*)-pteridinone, *in* A-60242
2-(Methylamino)purine, *in* A-60243
8-(Methylamino)purine, *in* A-60244
2-(Methylamino)-1*H*-pyrido[2,3-*b*]indole, *in* A-70105
5-Methylamino-1*H*-tetrazole, *in* A-70202
2-*O*-Methylangolensin, *in* A-80155
4-*O*-Methylangolensin, *in* A-80155
2-Methyl-*p*-anisaldehyde, *in* H-70161
5-Methylapionol, *see* M-80050
Methylarbutin, *in* A-70248
Methylarbutoside, *in* A-70248
3-Methylaspartic acid, *see* A-70166
Methyl aspartylphenylalanine, *see* A-60311
4-Methylayapin, *see* M-70092
▷ 8-Methyl-8-azabicyclo[3.2.1]octan-1-ol, *see* P-60151
2-Methyl-4-azaindole, *see* M-80157
2-Methyl-5-azaindole, *see* M-80159
2-Methyl-6-azaindole, *see* M-80158
2-Methyl-7-azaindole, *see* M-80156
6-Methyl-5-azauracil, *see* M-60132
4-Methyl-1-azulenecarboxylic acid, M-60042
1-Methylazupyrene, M-60043
9*b*-Methyl-9*bH*-benz[*cd*]azulene, M-60044
N-Methylbenzenecarboximidic acid, M-60045
2-Methyl-1,3-benzenedicarboxaldehyde, M-60046
2-Methyl-1,4-benzenedicarboxaldehyde, M-60047
4-Methyl-1,2-benzenedicarboxaldehyde, M-60048
4-Methyl-1,3-benzenedicarboxaldehyde, M-60049
5-Methyl-1,3-benzenedicarboxaldehyde, M-60050
2-Methyl-1,3-benzenedimethanethiol, M-70050
α-Methylbenzeneethanesulfonic acid, *see* P-70068
3-Methyl-1,2,4,5-benzenetetrol, M-80048
4-Methyl-1,2,3,5-benzenetetrol, M-80049
5-Methyl-1,2,3,4-benzenetetrol, M-80050
N-Methylbenzimidic acid, *see* M-60045
8-Methyl-6*H*-1,3-benzodioxolo[4,5-*g*][1]benzopyran-6-one, *see* M-70092
3-Methyl-4,5-benzofurandione, M-70051
α-Methylbenzoin, *see* H-70123
2-Methylbenzo[*gh*]perimidine, M-60051
3-Methyl-1*H*-2-benzopyran-1-one, M-70052
3-Methyl-2*H*-1-benzothiin, *see* M-80051
3-Methyl-2*H*-1-benzothiopyran, M-80051
4-Methyl-1,2,3-benzotriazine, M-80052
1-Methyl-8*H*-benzo[*cd*]triazirino[*a*]indazole, M-60052
2-Methyl-1,3-benzoxathiazolium(1+), M-80053
Methyl 3-benzoyloxyacrylate, *in* O-60090
Methyl 1-benzyl-1*H*-1,2,3-triazole-5-carboxylate, *in* T-60239
3-Methylbicyclo[1.1.0]butane-1-carboxylic acid, M-70053
5-*O*-Methylbiochanin A, *in* T-80309
7-*O*-Methylbiochanin A 6-*C*-rhamnoside, *see* I-80098
3-Methylbiphenyl, M-60053
3-Methyl-[1,1′-biphenyl]-2-amine, *see* A-70164
3-Methyl-2-biphenylamine, *see* A-70164
1′-Methyl-1,5′-bi-1*H*-pyrazole, *in* B-60119
2-Methyl-*N*,*N*-bis(2-methylphenyl)benzenamine, *see* T-70288
3-Methyl-*N*,*N*-bis(3-methylphenyl)benzenamine, *see* T-70289
4-Methyl-*N*,*N*-bis(4-methylphenyl)benzenamine, *see* T-70290
4-[5′-Methyl[2,2′-bithiophen]-5-yl]-3-butyne-1,2-diol, M-70054
Methyl 3-(3-bromo-4-chloro-4-methylcyclohexyl)-4-oxo-2-pentenoate, M-60054
2-Methylbutane-1,1-dicarboxylic acid, *see* M-70119
2-Methyl-1,3-butanediol, M-80054
3-Methyl-1,2-butanediol, M-80055
2-Methylbutanoic acid 2-amino-4-methoxy-1,5-dimethyl-6-oxo-2,4-cyclohexadien-1-yl ester, *see* W-70002
3-Methyl-4-butanolide, *see* D-80220
2-Methyl-2-butenal, M-80056
▷ 3-Methyl-2-butenal, M-70055
2-Methyl-2-buten-1-ol, M-80057
8-(3-Methyl-2-butenoyl)coumarin, *in* M-80190
6-(3-Methyl-2-butenyl)allopteroxylin, *in* A-60075
6-(3-Methyl-2-butenyl)allopteroxylin methyl ether, *in* A-60075
1-Methyl-1-butenylbenzene, *see* P-80119
2-(3-Methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,6*a*,9(11*aH*)triol, *see* G-80028
3-(3-Methyl-2-butenyl)furo[2,3,4-*de*]-1-benzopyran-2(5*H*)-one, *see* C-60214
Methyl 3-*tert*-butylamino-2-formyl-2-propenoate, *in* A-80134
Methyl *sec*-butyl ketone, *see* M-70105
▷ 3-[(3-Methylbutyl)nitrosoamino]-2-butanone, M-60055
3-Methyl-γ-butyrolactone, *see* D-80220
2′-*O*-Methylcajanone, *in* C-80009
9-Methyl-9*H*-carbazole, M-60056
N-Methylcarbazole, *see* M-60056
9-Methyl-9*H*-carbazol-2-ol, *in* H-60109
3-Methyl-6-carboxy-2-pyridone, *see* D-80225
5-Methyl-6-carboxy-2-pyridone, *see* D-80226
Methylcatalpol, *in* C-70026
Methyl 5-chloro-4-*O*-*demethylbarbatate*, *in* B-70007
Methyl 2-(3-chloro-2,6-dihydroxy-4-methylbenzoyl)-5-hydroxy-3-methoxybenzoate, *in* S-70083
▷ 6-Methylcholanthrene, M-70056
24-Methyl-7,22-cholestadiene-3,6-diol, M-80058
24-Methyl-7,22-cholestadiene-3,5,6-triol, M-70057
24-Methyl-7,22-cholestadien-3-ol, M-80059
4-Methylcholesta-8,14-dien-23-ol, M-80060
24-Methyl-7,22-cholestadien-3-one, *in* M-80059
24-Methyl-5,22,25-cholestatrien-3-ol, M-60057
24-Methyl-7-cholestene-3,5,6-triol, M-80061
2-Methylcrotonaldehyde, *see* M-80056

3-Methylcrotonaldehyde, *see* M-70055
1-(β-Methylcrotonoyloxy)-5-benzoyl-2,4-pentadiyne, *in* H-80235
Methyl 1-cyanocyclopropanecarboxylate, *in* C-80196
2-Methyl-4-cyanopyrrole, *in* M-60125
3-Methyl-3-cyclobutene-1,2-dione, M-80062
1-(2-Methyl-1-cyclobuten-1-yl)ethanone, *see* A-80028
Methyl-α-cyclohallerin, *in* C-60193
Methyl-β-cyclohallerin, *in* C-60193
3-Methyl-3,5-cyclohexadiene-1,2-diol, M-80063
α-Methylcyclohexaneacetaldehyde, *see* C-80184
3-Methyl-1,2-cyclohexanediol, M-80064
α-Methyl-1-cyclohexene-1-acetaldehyde, *see* C-80183
1-Methylcyclohexene oxide, *see* M-80125
1-Methyl-2-cyclohexen-1-ol, M-80065
6-Methyl-2-cyclohexen-1-ol, M-70058
4-Methyl-2-cyclohexen-1-one, M-80066
6-Methyl-2-cyclohexen-1-one, M-70059
9-Methylcyclolongipesin, *in* C-60214
Methylcyclononane, M-60058
2-Methylcyclooctanone, M-60059
11*b*-Methyl-11*bH*-Cyclooct[*cd*]azulene, M-60060
3-Methyl-1-cyclopentenecarboxaldehyde, M-80067
1-Methylcyclopentene oxide, *see* M-80126
1-(2-Methyl-1-cyclopenten-1-yl)ethanone, *see* A-60043
23-(2-Methylcyclopropyl)-24-norchola-5,22-dien-3-ol, *see* P-60004
O-Methyldehydrodieugenol, *in* D-80023
3-*O*-Methyl-2,5-dehydrosenecioodentol, *in* S-60022
2-*O*-Methyl-1,4-dehydrosenecioodontol, *in* S-60022
O^5-Methyl-3′,4′-deoxypsorospermin-3′-ol, *in* D-60021
4′-*O*-Methylderrone, *in* D-80031
Methyl 15α,17β-diacetoxy-6α-butanoyloxy-15,16-dideoxy-15,17-oxido-16-spongianate, *in* T-60038
Methyl 15α,17β-diacetoxy-15,16-dideoxy-15,17-oxido-16-spongianoate, *in* T-60038
2-Methyl-1,3-diazapyrene, *see* M-60051
Methyl 3,5-dichlorolecanorate, *see* T-70334
Methyl dicyanoacetate, *in* D-70149
1-Methyldicyclopenta[*ef*,*kl*]heptalene, *see* M-60043
Methyl 12,17;15,16-diepoxy-6-hydroxy-19-nor-17-oxo-4,13(16),14-clerodatrien-18-oate, M-80068
Methyl 3,3-diethoxypropionate, *in* O-60090
Methyl diformylacetate, *in* D-60190
3-*O*-Methyldihydrofusarubin A, *in* F-60108
Methyl 3,4-dihydro-8-isopropyl-5-methyl-2-naphalenecarboxylate, *in* I-60129
2-Methyl-1,4-dihydropyrimidine, *see* D-70225
2-Methyl-1,6-dihydropyrimidine, *see* D-70225
1-Methyl-1,2-dihydro-3*H*-pyrrol-3-one, *in* D-70262
2-Methyl-3,4-dihydroxybutanoic acid 1,4-lactone, *see* D-80214
Methyl 2-(2,6-dihydroxy-4-methylbenzoyl)-5-hydroxy-3-methoxybenzoate, *see* S-70083
Methyl 11,12-dimethoxy-6,8,11,13-abietatrien-20-oate, *in* D-60305
Methyl 2,2′-di-*O*-methyleriodermate, *in* E-70032
▷ 2-Methyl-1,3-dinitrobenzene, M-60061
1-Methyl-2,3-dinitro-1*H*-pyrrole, *in* D-60461
1-Methyl-2,4-dinitro-1*H*-pyrrole, *in* D-60462
1-Methyl-2,5-dinitro-1*H*-pyrrole, *in* D-60463
1-Methyl-3,4-dinitro-1*H*-pyrrole, *in* D-60464
2-Methyl-1,6-dioxaspiro[4.5]decane, M-60062
7-Methyl-1,6-dioxaspiro[4.5]decane, M-80069
▷ 2-Methyl-1,3-dioxolane, M-60063
5-Methyl-3,6-dioxo-2-piperazineacetic acid, M-60064
N-Methyldiphenylamine, M-70060
1-Methyl-4,4-diphenylcyclohexene, M-60065
3-Methyl-4,4-diphenylcyclohexene, M-60066
2-Methyl-1,5-diphenyl-1*H*-pyrrole, *in* M-60115
2-Methyl-1,3-diselenole, M-80070
5-Methyl-1,3-dithiane, M-60067
5-Methyl-1,3,2,4-dithiazolium(1+), M-70061
▷ 5-Methyl-2,4-dithiouracil, *see* M-70127
6-Methyl-2,4-dithiouracil, *see* M-70128
2-Methyldotriacontane, M-80071
3-Methyldotriacontane, M-80072
6-Methyldotriacontene, M-80073
Methyleneadamantane, M-60068
2-Methylene-1-azabicyclo[2.2.2]octan-3-one, M-80074
N,*N*′-Methylene-2,2′-azapyridocyanine, *see* D-60495
α-Methylenebenzenemethanol, *see* P-60092
4-Methylenebicyclo[3.1.0]hex-2-ene, M-60069
7-Methylenebicyclo[3.3.1]nonan-3-one, M-70062
2-Methylenebicyclo[2.1.0]pentane, M-80075
2,2′-Methylenebis[6-acetyl-3,5-dihydroxy-4,4-dimethyl-2,5-cyclohexadien-1-one], *in* A-80043
2,2′-Methylenebis[6-*tert*-butyl-*p*-cresol], *see* M-80076
2,2′-Methylenebis[6-*tert*-butyl-4-methylphenol], M-80076
Methylenebisdesaspidinol BB, M-80077
1,1′-[Methylenebis(2,6-dihydroxy-4-methoxy-3,1-phenylene)]bis-1-butanone, *see* M-80077
2,2′-Methylenebis[6-(1,1-dimethylethyl)-4-methylphenol], *see* M-80076
3,3′-Methylenebis[4-hydroxy-5-methyl-2*H*-1-benzopyran-2-one], *see* G-60013
2,2′-Methylenebis[8-hydroxy-3-methyl-1,4-naphthalenedione], M-70063
2,2′-Methylenebis-1*H*-imidazole, M-70064
3,3′-Methylenebisindole, M-80078
2,2′-Methylenebispyridine, *see* D-60496
1,1′-Methylenebispyridinium(1+), M-70065
24-Methylene-1α,3β,5α,6β-cholestanetetrol, *see* N-80084
24-Methylene-5-cholestene-3,4,7,20-tetrol, M-60070
22-Methylene-3β-cycloartanol, *see* C-60232
Methylenecyclobutane, M-70066
Methylenecycloheptane, M-80079
4-Methylene-2,5-cyclohexadien-1-one, M-60071
6-Methylene-2,4-cyclohexadien-1-one, M-60072
2-Methylenecyclohexanone, M-80080
3-Methylenecyclohexanone, M-80081
4-Methylenecyclohexanone, M-80082
9-Methylene-1,3,5,7-cyclononatetraene, M-60073
7-Methylene-1,3,5-cyclooctatriene, M-60074
2-Methylene-1,3-cyclopentanedione, M-80083
2-Methylenecyclopropaneacetic acid, M-70067
[(Methylenecyclopropyl)sulfinyl]benzene, *in* M-80090
[(Methylenecyclopropyl)sulfonyl]benzene, *in* M-80090
[(Methylenecyclopropyl)thio]benzene, *see* M-80090
5-Methylene-5*H*-dibenzo[*a*,*d*]cycloheptene, M-80084
3-Methylenedibenzsuberane, *see* D-80219
1-Methylene-2,3:6,7-dibenz-4-suberene, *see* M-80084
3,3′-Methylenediindole, *see* M-80078
7-Methylene-1,4-dioxaspiro[4.5]decane, *in* M-80081
2-Methylene-1,3-dioxolane, M-60075
4-Methylene-1,3-dioxolane, M-60076
3,4-Methylenedioxybenzocyclobutene-1,2-dione, *in* D-80274
6,7-Methylenedioxy-2*H*-1-benzopyran-2-one, M-70068
6,7-Methylenedioxycoumarin, *see* M-70068
6-(3,4-Methylenedioxylphenyl)-1-hexene, *in* M-50261
3′,4′-Methylenedioxyorobol, *in* T-80109
2,3-Methylenedioxyphenylacetic acid, *see* B-60029
2,3-Methylenedioxyphenylacetonitrile, *in* B-60029
3-(3,4-Methylenedioxyphenyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, *see* C-60006
6-(3,4-Methylenedioxyphenyl)-2-hexanol, *in* M-50261
6-(3,4-Methylenedioxyphenyl)-2-hexanone, *see* M-50261
5-(3,4-Methylenedioxyphenyl)pentanoic acid, M-80085
1-(3,4-Methylenedioxyphenyl)-1-tetradecene, M-60077
1,2-(Methylenedioxy)-4-(1-propenyl)benzene, *see* I-80089
4,5-Methylenedioxysalicylaldehyde, *see* H-70175
6-(3,4-Methylenedioxystyryl)-α-pyrone, M-80086
3,3′-Methylenediplumbagin, *see* M-70063
1,1-Methylenedipyridinium, *see* M-70065
2-Methylene-1,3-diselenole, M-70069
3-Methyleneglutamic acid, *see* A-60219
2-Methyleneglutaronitrile, *see* M-80089
4-Methylene-1,2,5,6-heptatetraene, M-70070
(1-Methyleneheptyl)benzene, *see* P-80108
4-Methylene-1,2,5-hexatriene, M-70071
25-Methylene-22-homocholestane-1β,3β,5α-triol, *see* N-80085
1-Methyleneindane, M-60078
24-Methylene-7,9(11)-lanostadien-3-ol, M-70072
24-Methylene-8-lanostene-3,22-diol, M-80087
4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane, *see* T-80195
22-Methylene-30-nor-3β-cycloartanol, *see* N-60059
22-Methylene-30-nor-3-cycloartanone, *in* N-60059
2-Methylene-7-oxabicyclo[2.2.1]heptane, M-70073
4-Methylene-2-oxabicyclo[3.3.0]octan-3-one, *see* H-70062
2-Methylene-3-oxocyclobutanecarboxylic acid, M-80088
2-Methylenepentanedinitrile, M-80089
2-Methylene-4-pentenal, M-70074
3-Methylene-4-penten-2-one, M-70075
3-Methyleneperhydrobenzofuran-2-one, *see* H-70062
β-Methylenephenylalanine, *see* A-60238
1-Methylene-2-(phenylsulfinyl)cyclopropane, *in* M-80090
1-Methylene-2-(phenylsulfonyl)cyclopropane, *in* M-80090
1-Methylene-2-(phenylthio)cyclopropane, M-80090
2-Methylene-1,3-propanedithiol, M-70076
1-Methylenepyrrolidinium(1+), M-70077
2-Methylene-3-quinuclidinone, *see* M-80074
24-Methylene-3,4-seco-4(28)-cycloarten-3-oic acid, M-70078
4-Methylene-1,2,3,5-tetraphenylbicyclo[3.1.0]hex-2-ene, M-60079
11-Methylene-1,5,9-triazabicyclo[7.3.3]pentadecane, M-60080
Methylenetricyclo[3.3.1.1^{3,7}]decane, *see* M-60068
Methylene-1,3,5-trioxane, M-60081
Methylenolactocin, M-70079
Methyl 3,6-epidioxy-6-methoxy-4,16,18-eicosatrienoate, *in* E-60007
Methyl 3,6-epidioxy-6-methoxy-4,16-octadecadienoate, *in* E-60008

Methyl 3,6-epidioxy-6-methoxy-4,14,16-octadecatrienoate, *in* E-60008
Methyl 3,6-epidioxy-6-methoxy-4-octadecenoate, *in* E-60008
8β-(2-Methyl-2,3-epoxybutyroyloxy)-dehydroleucodin, *in* H-80184
Methyl 10,11-epoxy-3,7-diethyl-11-methyl-2,6-tridecadienoate, *see* J-80018
Methyl 14ξ,15-epoxy-8(17),12*E*-labdadien-16-oate, *in* E-60025
8β-(2-Methyl-2,3-epoxypropionyloxy)hirsutinolide, *in* H-80089
8β-(2-Methyl-2,3-epoxypropionyloxy)hirsutinolide 13-*O*-acetate, *in* H-80089
Methyl eriodermate, *in* E-70032
13^1-Methyl-13,15-ethano-13^2,17-prop-$13^2(15^2)$-enoporphyrin, M-60082
1-(1-Methylethenyl)cyclohexene, *see* I-60115
3-(1-Methylethenyl)cyclohexene, *see* I-60116
4-(1-Methylethenyl)cyclohexene, *see* I-60117
1-[4-(1-Methylethenyl)-1-cyclopenten-1-yl]ethanone, *see* A-80025
(1-Methylethenyl)oxirane, M-70080
[(1-Methylethenyl)thio]benzene, *see* P-80137
(1-Methylethoxy)benzene, *see* I-80085
5-Methylethuliacoumarin, *in* E-60045
3-(1-Methylethyl)aspartic acid, *see* A-70162
α-(1-Methylethyl)benzeneacetaldehyde, *see* M-70109
▷ 4-(1-Methylethyl)benzenemethanol, *see* I-80078
2-(1-Methylethyl)cycloheptanone, *see* I-70090
4-(1-Methylethyl)cycloheptanone, *see* I-70091
1-(1-Methylethyl)cyclohexene, *see* I-60118
3-(1-Methylethyl)cyclohexene, *see* I-60119
4-(1-Methylethyl)cyclohexene, *see* I-60120
(1-Methylethyl)cyclopentane, *see* I-70092
Methyl 2-ethyl-1,2,3,4,6,11-hexahydro-2,4,5,7,12-pentahydroxy-6,11-dioxo-1-naphthacenecarboxylate, *see* R-70002
β-Methyl-β-ethylhydracrylic acid, *see* H-80210
1-[4-(1-Methylethylidene)-1-cyclopenten-1-yl]ethanone, *see* A-80026
2-(1-Methylethylidene)tricyclo[3.3.1.$1^{3,7}$]decane, *see* I-60121
3-(1-Methylethyl)-2-naphthalenol, *see* I-70095
4-(Methylethyl)-1-naphthalenol, *see* I-70096
2-(1-Methylethyl)-1,3,5-trimethylbenzene, *see* I-60130
Methyl 4-fluoro-3,5-dimethoxybenzoate, *in* F-60024
▷ Methylfluoroform, *see* T-80273
2-Methyl-3-furanmethanol, *see* H-80207
▷ 5-Methyl-2(3*H*)-furanone, M-70081
▷ 5-Methyl-2(5*H*)-furanone, M-60083
▷ 2-Methyl-3-furanthiol, M-70082
2-Methylfuro[2,3-*b*]pyridine, M-60084
3-Methylfuro[2,3-*b*]pyridine, M-60085
2-Methylfuro[3,2-*c*]quinoline, M-70083
O-Methylganoderic acid *O*, *in* T-60111
▷ *Methylgenistein, *in* T-80309
5-*O*-Methylgenistein, *see* D-80336
Methyl *p*-geranyloxycinnamate, *in* H-80242
4′-*O*-Methylglabridin, *in* G-70016
4-Methylglutamic acid, *see* A-60223
γ-Methylglutamic acid, *see* A-60223
2-Methylglyceric acid, *see* D-60312
2-Methylglycidic acid, *see* M-80127
1-*O*-Methylglycyrol, *in* P-80186
5-*O*-Methylglycyrol, *in* P-80186
1-Methylguanosine, M-70084
8-Methylguanosine, M-70085
O-Methylhaenkeanoside, *in* H-80001
2-Methylheneicosane, M-80091
3-Methylheptacosane, M-80092
3-Methyl-2-heptenoic acid, M-60086
3-Methyl-4-hepten-2-one, M-80093
4-Methyl-3-hepten-2-one, M-60087
6-Methyl-6-hepten-2-one, M-80094
2-Methylhexacosane, M-80095
5-Methyl-2,4-hexadienoic acid, M-70086
5-Methyl-3,4-hexadienoic acid, M-70087
Methyl 2-(2,4-hexadiynyl)-6-methoxybenzoate, *see* F-80084
2-Methylhexanedial, M-80096
4-Methyl-3-hexanone, M-80097
2-Methyl-4-hexenal, M-80098
5-Methyl-4-hexen-1-amine, M-80099
2-Methyl-4-hexenoic acid, M-80100
4-Methyl-2-hexenoic acid, M-80101
2-Methyl-4-hexen-1-ol, M-80102
2-Methyl-4-hexen-2-ol, M-80103
2-Methyl-5-hexen-1-ol, M-80104
3-Methyl-5-hexen-1-ol, M-80105
4-Methyl-2-hexen-1-ol, M-80106
4-Methyl-3-hexen-2-ol, M-80107
4-Methyl-4-hexen-1-ol, M-80108
4-Methyl-4-hexen-2-ol, M-80109
4-Methyl-5-hexen-1-ol, M-80110
5-Methyl-4-hexen-2-ol, M-80111
5-Methyl-4-hexen-3-ol, M-80112
5-Methyl-5-hexen-1-ol, M-80113
5-Methyl-5-hexen-3-ol, M-80114
3-Methyl-4-hexen-2-one, M-80115
1-Methyl-1-hexenylbenzene, *see* P-80102
Methylhomoserine, *see* A-60186
7-*O*-Methylhorminone, *in* D-80265
p-Methylhydratropic acid, *see* M-60114
Methylhydrocotoin, *in* T-80285
Methyl hydrogen 2-formylmalonate, *in* H-80204
Methyl hydrogen 2-(*tert*-butoxymethyl)-2-methylmalonate, M-70088
Methyl hydrogen 3-hydroxyglutarate, M-70089
Methyl 2-[(2-hydroxybenzoyl)amino]-4-hydroxybenzoate, *in* D-70049
Methyl hydroxycarbamate, *see* M-70044
7-Methylidenebicyclo[3.3.1]nonan-3-one, *see* M-70062
1-Methylidene-2-(phenylsulfinyl)cyclopropane, *in* M-80090
1-Methylidene-2-(phenylsulfonyl)cyclopropane, *in* M-80090
1-Methylidene-2-(phenylthio)cyclopropane, *see* M-80090
6-Methylidenetetrahydro-2-pyrone, *see* T-70074
1,1′,1″-Methylidynetris[2,3,4,5,6-pentachlorobenzene], *see* T-60405
6-Methyl-1*H*-indole, M-60088
3-Methyl-1*H*-indole-2-carboxaldehyde, M-70090
Methyl 2-iodo-3,5-dimethoxybenzoate, *in* D-60336
Methyl 4-iodo-3,5-dimethoxybenzoate, *in* D-60337
3-Methylisocoumarin, *see* M-70052
6-Methylisocytosine, *see* A-60230
▷ Methylisogenistin, *in* T-80309
1-Methylisoguanosine, *see* D-60518
O-Methylisohaenkeanoside, *in* H-80001
Methylisohallerin, *in* I-60100
2-Methylisophthalaldehyde, *see* M-60046
4-Methylisophthalaldehyde, *see* M-60049
5-Methylisophthalaldehyde, *see* M-60050
Methyl 8-isopropyl-5-methyl-2-naphthalenecarboxylate, *in* I-60129
2′-*O*-Methylisopseudocyphellarin A, *in* I-70098
1-Methyl-3-isoquinolinamine, *see* A-80099
1-Methyl-4-isoquinolinamine, *see* A-80101
1-Methyl-5-isoquinolinamine, *see* A-80102
1-Methyl-7-isoquinolinamine, *see* A-80104
1-Methyl-8-isoquinolinamine, *see* A-80105
3-Methyl-1-isoquinolinamine, *see* A-80098
3-Methyl-5-isoquinolinamine, *see* A-80103
4-Methyl-3-isoquinolinamine, *see* A-80100
Methylisoselenourea hydrogen sulfate, *in* S-70031
Methylisoselenourea iodide, *in* S-70031
3-Methylisoserine, *see* A-60183
3-Methyl-4-isoxazolamine, *see* A-80107
4-Methyl-3-isoxazolamine, *see* A-80106
4-Methyl-5-isoxazolamine, *see* A-80109
5-Methyl-4-isoxazolamine, *see* A-80108
5-Methyl-4-isoxazolecarboxylic acid, M-80117
Methyl jasmonate, *in* J-60002
Methyllanceolin, *in* P-60052
4-Methylleucine, *see* A-70137
Methyllinderatin, *in* L-50048
Methyllinderatone, *in* L-70030
9-Methyllongipesin, M-70091
3′-*O*-Methyllutonarin, *in* I-80068
▷ Methylmalonic acid, *see* M-80149
Methylmalononitrile, *in* M-80149
α-Methylmandelaldehyde, *see* H-80240
1-Methyl-4-mercaptohistidine, *see* O-70050
Methyl 3-(4-methoxy-2-vinylphenyl)propanoate, *in* H-70232
Methyl 3-formyl-3-methylacrylate, *in* M-70103
1-Methyl-4-methylamino-5-(methylaminocarbonyl)imidazole, *see* C-60003
Methyl 2-formyl-3-methylamino-2-propenoate, *in* A-80134
1-Methyl-5-methylamino-1*H*-tetrazole, *in* A-70202
2-Methyl-5-methylamino-2*H*-tetrazole, *in* A-70202
2-Methyl-6-(4-methylenebicyclo[3.1.0]hex-1-yl)-2-heptenal, *in* S-70037
4-Methyl-6,7-methylenedioxy-2*H*-1-benzopyran-2-one, M-70092
4-Methyl-6,7-methylenedioxycoumarin, *see* M-70092
4-(5-Methyl-1-methylene-4-hexenyl)-1-(4-methyl-3-pentenyl)cyclohexene, *see* C-70009
4-Methyl-10-methylene-7-(1-methylethyl)-5-cyclodecene-1,4-diol, *see* G-70009
2-Methyl-6-methylene-2,7-octadien-4-ol, M-70093
7-Methyl-3-methylene-1-octanol, M-80118
2-Methyl-6-methylene-1,3,7-octatriene, M-60089
2-Methyl-6-methylene-7-octen-4-ol, *in* M-70093
4-Methyl-3-methylene-2-oxetanone, M-80119
Methyl 2-*O*-methyleriodermate, *in* E-70032
Methyl 2′-*O*-methyleriodermate, *in* E-70032
Methyl 4-*O*-methyleriodermate, *in* E-70032
1-Methyl-4-(1-methylethenyl)-1,2-cyclohexanediol, *see* I-70086
3-Methyl-6-(1-methylethenyl)-2-cyclohexen-1-one, *see* I-70088
3-Methyl-6-(1-methylethenyl)-9-decen-1-ol, *see* I-70089
5-Methyl-8-(1-methylethenyl)-10-oxabicyclo[7.2.1]dodeca-1(12),4-dien-11-one, *see* A-60296
3-Methyl-2-[2-(1-methylethenyl)-5-oxohexyl]-2-cyclopenten-1-one, *see* M-80004
2-Methyl-5-(1-methylethyl)-1,3-benzenediol, *see* I-60125
2-Methyl-6-(1-methylethyl)-1,4-benzenediol, *see* I-60123
3-Methyl-5-(1-methylethyl)-1,2-benzenediol, *see* I-60126
3-Methyl-6-(1-methylethyl)-1,2-benzenediol, *see* I-60124
4-Methyl-5-(1-methylethyl)-1,3-benzenediol, *see* I-60127
5-Methyl-2-(1-methylethyl)-1,3-benzenediol, *see* I-60122
2-Methyl-5-(1-methylethyl)bicyclo[3.1.0.]hex-2-ene, *see* T-80194
1-Methyl-4-(1-methylethyl)-3-cyclohexane-1,2-diol, *see* I-70093
1-Methyl-4-(1-methylethyl)-4-cyclohexene-1,2-diol, *see* I-70094
1-Methyl-4-(1-methylethyl)-4-cyclohexene-1,2-diol, *see* M-80014
2-Methyl-5-(1-methylethyl)furan, *see* I-80083

7-Methyl-3-(1-methylethyl)-8-(4-methyl-3-pentenyl)-1,2-naphthalenedione, *see* S-80010
5-Methyl-8-(1-methylethyl)-2-naphthalenecarboxaldehyde, *see* I-60129
7-Methyl-4-(1-methylethyl)-1-naphthalenecarboxaldehyde, *see* I-80084
6-Methyl-3-(1-methylethyl)-7-oxabicyclo[4.1.0]heptan-2-one, *see* P-80153
1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)cyclohexene, *see* B-80134
2-Methyl-5-[2-methyl-5-(5-oxo-2*H*-furan-3-yl)-2-pentenyl]-2(5*H*)-furanone, *see* F-80001
5-Methyl-2-(1-methyl-1-phenylethyl)cyclohexanol, M-60090
Methyl 4-methylphenyl sulfoxide, M-70094
3-Methyl-6-(1-methyl-1-propenyl)-2*H*-pyran-2-one, *see* F-80099
1-Methyl-4-(methylsulfinyl)benzene, *see* M-70094
1-Methyl-2-methylthio-1*H*-imidazo[4,5-*b*]pyrazine, *in* D-60247
4-Methyl-2-methylthio-4*H*-imidazo[4,5-*b*]pyrazine, *in* D-60247
2-Methyl-6-(methylthio)-3(2*H*)-pyridazinethione, *in* M-80028
1-Methyl-4-(methylthio)-2(1*H*)-pyridinethione, *in* M-80029
1-Methyl-4-(methylthio)-2(1*H*)-pyridinethione, *in* P-60219
3-Methyl-5-(methylthio)-1,3,4-thiadiazole-2(3*H*)-thione, *in* M-70031
Methyl 1-methyl-1*H*-1,2,3-triazole-5-carboxylate, *in* T-60239
2′-*O*-Methylmicrophyllinic acid, *in* M-70147
3-Methyl-1-naphthaldehyde, M-80120
5-Methyl-1-naphthaldehyde, M-80121
3-Methyl-1-naphthalenecarboxaldehyde, *see* M-80120
5-Methyl-1-naphthalenecarboxaldehyde, *see* M-80121
2-Methyl-1,3-naphthalenediol, M-60091
2-Methyl-1,5-naphthalenediol, M-60092
3-Methyl-1,2-naphthalenediol, M-60093
4-Methyl-1,3-naphthalenediol, M-60094
6-Methyl-1,2-naphthalenediol, M-60095
α-Methyl-1-naphthaleneethanol, *see* N-60015
α-Methyl-1-naphthalenemethanol, *see* N-70015
1-Methylnaphtho[2,1-*b*]thiophene, M-60096
2-Methylnaphtho[2,1-*b*]thiophene, M-60097
4-Methylnaphtho[2,1-*b*]thiophene, M-60098
5-Methylnaphtho[2,1-*b*]thiophene, M-60099
6-Methylnaphtho[2,1-*b*]thiophene, M-60100
7-Methylnaphtho[2,1-*b*]thiophene, M-60101
8-Methylnaphtho[2,1-*b*]thiophene, M-60102
9-Methylnaphtho[2,1-*b*]thiophene, M-60103
2-Methyl-2*H*-naphtho[1,8-*de*]triazine, M-70095
2-Methyl-1*H*-naphtho[1,8-*de*]-1,2,3-triazinium hydroxide inner salt, *see* M-70095
Methyl-1-naphthylcarbinol, *see* N-70015
7-Methylnapyradiomycin *A*, *see* A-70237
2-Methylnebularine, *see* M-70130
6-Methylnebularine, *see* M-70131
5-Methylnicotinaldehyde, *see* M-80152
Methyl nidoresedate, *in* N-70035
Methylnimbiol, *in* N-80027
Methyl nimbionone, *in* D-80374
Methylnissolin, *in* T-80338
2-Methyl-4-nitrobenzaldehyde, M-70096
2-Methyl-4-nitro-1,3-benzenediol, M-70097
3-Methyl-2-nitrobiphenyl, M-70098
3-Methyl-1-nitrocyclopentene, M-80122
▷ *N*-Methyl-*N*-nitromethanamine, *see* N-80045
3-Methyl-4-nitropyridine, M-70099
4-Methyl-5-nitropyrimidine, M-60104
2-Methyl-4-nitroresorcinol, *see* M-70097
▷ 1-Methyl-2-nitroso-1*H*-imidazole, *in* N-80059
3-Methyl-4-nonanolide, *see* D-80227
24-Methyl-27-nor-7,22-cholestadiene-3,6-diol, M-80123
24-Methyl-25-nor-12,24-dioxo-16-scalaren-22-oic acid, M-60105
8-*O*-Methylochramycinone, *in* O-60003
2-Methyloctacosane, M-80124
2-Methyl-1-(octahydro-3,7-dimethyl-4*H*-inden-1-ylidene)-2-propanol, *see* V-80001
2-Methyl-2-octenal, M-60106
2-Methylornithine, *see* D-80061
3′-*O*-Methylorobol, *in* T-80109
1-Methyl-7-oxabicyclo[4.1.0]heptane, M-80125
1-Methyl-6-oxabicyclo[3.1.0]hexane, M-80126
16-Methyloxacyclohexadecan-2-one, *in* H-80173
14-Methyloxacyclotetradec-6-en-2-one, *see* T-80045
5-Methyl-2-oxazolidinone, M-60107
10-Methyl-2-oxecanone, *in* H-80149
▷ Methyloxirane, M-70100
3-Methyloxiranecarboxylic acid, M-80127
3-Methyloxiranemethanol, M-80128
5-(2-Methyloxiranyl)benzofuran, M-70101
α-Methyl-γ-oxobenzenebutanoic acid, *see* B-60064
α-Methyl-β-oxobenzenepropanal, *see* B-80057
2-Methyl-3-oxobutanal, M-70102
3-Methyl-2-oxobutanenitrile, *in* M-80129
3-Methyl-2-oxobutanoic acid, M-80129
3-Methyl-4-oxo-2-butenoic acid, M-70103
6-Methyl-7-(3-oxobutyl)-2-cyclohepten-1-one, *see* C-60153
4-(1-Methyl-3-oxobutyl)-1-cyclohexene-1-carboxylic acid, *see* L-80025
Methyl 3-oxo-1,4(15),11(13)-eudesmatrien-12-oate, *in* H-80164
6-Methyl-5-oxoheptanoic acid, M-80130
Methyl 7-oxo-8(14),15-isopimaradien-18-oate, *in* O-70094
Methyl 4-oxonorpinguisan-12-oate, *in* N-80083
5-Methyl-2-oxo-4-oxazolidinecarboxylic acid, M-60108
3-Methyl-4-oxo-2-pentenal, M-70104
3-Methyl-4-[(5-oxo-3-phenyl-2-pyrazolin-4-ylidene)methyl]-1-phenyl-2-pyrazolin-5-one, *see* P-70153
3-Methylpentacosane, M-80131
5-Methyl-5-pentacosanol, M-80132
2-Methyl-1,3-pentadiene, M-80133
4-Methyl-1,3-pentadiene-1-carboxylic acid, *see* M-70086
3-Methylpentane-1,2-dicarboxylic acid, *see* M-80150
3-Methyl-5-pentanolide, *in* H-70182
3-Methyl-2-pentanone, M-70105
▷ 4-Methyl-2-pentanone, M-60109
▷ 2-Methyl-2-pentenal, M-70106
4-Methyl-4-pentenal, M-80134
2-Methyl-4-penten-1-ol, M-80135
4-Methyl-1-penten-3-ol, M-70107
2′-*O*-Methylphaseollidinisoflavan, *in* P-80077
Methyl *N*-phenacylcarbamate, *in* O-70099
3-Methylphenanthrene, M-70108
2′-*O*-Methylphenarctin, *in* P-70054
3-Methyl-1-phenazinecarboxylic acid, M-80136
4-Methyl-1-phenazinecarboxylic acid, M-80137
6-Methyl-1-phenazinecarboxylic acid, M-80138
7-Methyl-1-phenazinecarboxylic acid, M-80139
8-Methyl-1-phenazinecarboxylic acid, M-80140
9-Methyl-1-phenazinecarboxylic acid, M-80141
1-Methyl-2-phenyl-4(1*H*)-*quinolinone*, *in* P-60132
N-Methylphenylacetohydroxamic acid, *in* P-70059
2-Methyl-3-phenylalanine, *see* A-60225
α-Methylphenylalanine, *see* A-60225
Methyl 2-formyl-3-phenylamino-2-propenoate, *in* A-80134
N-Methyl-*N*-phenylbenzenamine, *see* M-70060
α-Methyl-α-phenylbenzeneacetic acid, *see* D-70493
β-Methyl-α-phenylbenzenepropanoic acid, *see* D-80506
5-Methyl-2-phenyl-1,5-benzothiazepin-4(5*H*)-one, *in* P-60081
1-Methyl-4-phenyl-1λ^4-1-benzothiopyran-2-carbonitrile, M-80142
3-Methyl-2-phenylbutanal, M-70109
2-Methyl-4-phenyl-3-butyn-2-ol, M-70110
3-Methyl-3-phenylcyclopentanone, M-80143
β-Methyl-α-phenylhydrocinnamic acid, *see* D-80506
1-Methyl-2-phenyl-1*H*-imidazole-4-carboxaldehyde, *in* P-60111
1-Methyl-2-phenyl-1*H*-imidazole-5-carboxaldehyde, *in* P-60111
▷ Methyl phenyl ketone, *see* A-60017
3-Methyl-8-phenyl-3,5,7-octatrien-2-one, M-80144
5-Methyl-3-phenyl-1,2,4-oxadiazole, M-60110
2-Methyl-5-phenyloxazole, M-80145
4-Methyl-5-phenyl-2-oxazolidinethione, M-60111
5-Methyl-3-phenyl-2-oxazolidinone, *in* M-60107
4-(4-Methylphenyl)-2-pentanone, M-60112
2-(2-Methylphenyl)propanoic acid, M-60113
2-(4-Methylphenyl)propanoic acid, M-60114
2-Methyl-1-phenyl-2-propen-1-one, M-80146
3-Methyl-1-phenylpyrazole-4,5-dione 4-(2,5-dichlorophenyl)hydrazone, *see* D-70138
2-Methyl-4-phenylpyrimidine, M-70111
2-Methyl-5-phenylpyrimidine, M-70112
4-Methyl-2-phenylpyrimidine, M-70113
4-Methyl-5-phenylpyrimidine, M-70114
4-Methyl-6-phenylpyrimidine, M-70115
5-Methyl-2-phenylpyrimidine, M-70116
5-Methyl-4-phenylpyrimidine, M-70117
▷ 2-Methyl-5-phenyl-1*H*-pyrrole, M-60115
2-Methyl-5-phenylpyrrolidine, M-80147
1-Methyl-3-phenyl-2,5-pyrrolidinedione, *in* P-80132
Methyl phenyl sulfoximine, M-80148
▷ 1-Methyl-4-phenyl-1,2,3,6-tetrahydropyridine, *in* T-60081
4-Methyl-5-phenyl-1,2,3-thiadiazole, M-60116
5-Methyl-4-phenyl-1,2,3-thiadiazole, M-60117
6-Methyl-3-phenyl-1,2,4-triazine, M-60118
4-*O*-Methylphloracetophenone, *in* T-70248
4-Methylphthalaldehyde, *see* M-60048
α-Methylpipecolic acid, *see* M-60119
2-Methyl-2-piperidinecarboxylic acid, M-60119
O-Methylpisiferic acid, *see* M-60036
3′-*O*-Methylpratensein, *in* T-80109
2-Methylproline, *see* M-60126
N-Methylproline methylbetaine, *see* S-60050
Methylpropanedinitrile, *in* M-80149
▷ Methylpropanedioic acid, M-80149
2-Methyl-1,3-propanediol, M-60120
2-Methyl-1,3-propanedithiol, M-60121
2-Methyl-2-propanesulfinic acid, *see* B-80293
4-[3-Methyl-5-(1-propenyl)-2-benzofuranyl]phenol, *see* E-60075
(1-Methylpropyl)butanedioic acid, M-80150
3-(2-Methylpropyl)-6-methyl-2,5-piperazinedione, M-70118
2-Methyl-4-propyl-1,3-oxathiane, M-60122
(1-Methylpropyl)propanedioic acid, M-70119
N-Methylprotoporphyrin IX, M-60123
2′-*O*-Methylpseudocyphellarin A, *in* P-70127
4′-*O*-Methylpsorospermindiol, *in* P-70133
5-*O*-Methylpsorospermindiol, *in* P-70133
2-Methylpteridine, M-70120
4-Methylpteridine, M-70121
6-Methylpteridine, M-70122
7-Methylpteridine, M-70123
9-Methyl-9*H*-purin-8-amine, *in* A-60244
7-Methyl-7*H*-purin-6-amine, *see* A-60226
2-Methyl-4-(1*H*-purin-6-ylamino)-2-penten-1-ol, *see* M-60133

6-Methyl-3-pyridazinol, *in* M-70124
6-Methyl-4-pyridazinol, *see* M-80151
6-Methyl-3-pyridazinone, M-70124
4-Methyl-3(2*H*)-pyridazinone, M-70125
5-Methyl-3(2*H*)-pyridazinone, M-70126
6-Methyl-4(1*H*)-pyridazinone, M-80151
5-Methyl-3-pyridinecarboxaldehyde, M-80152
α-Methyl-α-2-pyridinylisoquinolinemethanol, *see* I-60134
6-Methyl-4(1*H*)-pyridone-3-carboxylic acid, *see* D-80224
▷ 5-Methyl-2,4-(1*H*,3*H*)-pyrimidinedithione, M-70127
6-Methyl-2,4(1*H*,3*H*)-pyrimidinedithione, M-70128
Methyl 2-pyrimidinyl ketone, *see* A-60044
Methyl 4-pyrimidinyl ketone, *see* A-60045
Methyl 5-pyrimidinyl ketone, *see* A-60046
5-Methyl-1*H*-pyrrole-2-carboxaldehyde, M-70129
5-Methyl-1*H*-pyrrole-2-carboxylic acid, M-60124
5-Methyl-1*H*-pyrrole-3-carboxylic acid, M-60125
2-Methyl-2-pyrrolidinecarboxylic acid, M-60126
3-Methyl-2,5-pyrrolidinedione, M-80155
2-Methyl-1-pyrroline, *see* D-70226
2-Methyl-1*H*-pyrrolo[2,3-*b*]pyridine, M-80156
2-Methyl-1*H*-pyrrolo[3,2-*b*]pyridine, M-80157
2-Methyl-1*H*-pyrrolo[2,3-*c*]pyridine, M-80158
2-Methyl-1*H*-pyrrolo[3,2-*c*]pyridine, M-80159
Methyl 3-pyrryl ketone, *see* A-70052
2-Methyl-4,5,8-quinazolinetrione, M-80160
5-Methyl-5*H*-quindoline, *in* I-70016
Methyl 2-quinolinyl ketone, *see* A-60049
Methyl 3-quinolinyl ketone, *see* A-60050
Methyl 4-quinolinyl ketone, *see* A-60051
Methyl 5-quinolinyl ketone, *see* A-60052
Methyl 6-quinolinyl ketone, *see* A-60053
Methyl 7-quinolinyl ketone, *see* A-60054
Methyl 8-quinolinyl ketone, *see* A-60055
Methyl 2-quinoxalinyl ketone, *see* A-60056
Methyl 5-quinoxalinyl ketone, *see* A-60057
Methyl 6-quinoxalinyl ketone, *see* A-60058
8-*O*-Methylretusin, *in* T-80311
1-Methyl-9-β-D-ribofuranosylguanine, *see* M-70084
8-Methyl-9-β-D-ribofuranosylguanine, *see* M-70085
2-Methyl-9-β-D-ribofuranosyl-9*H*-purine, M-70130
6-Methyl-9-β-D-ribofuranosyl-9*H*-purine, M-70131
Methylripariochromene A, *in* A-80023
Methylsainfuran, *in* S-60002
4-Methylsalicylaldehyde, *see* H-70160
Methyl *N*-salicyl-4-hydroxyanthranilate, *in* D-70049
4-Methylsalicylic acid, *see* H-70163
[2-(Methylseleninyl)ethenyl]benzene, *in* M-70132
Methyl selenocyanate, M-60127
[2-(Methylseleno)ethenyl]benzene, M-70132
[2-(Methylselenonyl)ethenyl]benzene, *in* M-70132
2-(Methylseleno)pyridine, *in* P-70170
3-*O*-Methylsenecioodentol, *in* S-60022
2′-*O*-Methylsepiol, *in* T-80103
5-Methylsorbic acid, *see* M-70086
Methyl styryl selenide, *see* M-70132
Methyl styryl selenoxide, *in* M-70132
Methyl styryl sulfide, *see* M-80170
Methyl styryl sulfone, *in* M-80170
(*E*)-Methylsuberenol, *in* S-70080
(*Z*)-Methylsuberenol, *in* S-70080
2-Methylsuccinimide, *see* M-80155
2-(Methylsulfinyl)adamantane, *in* A-80038
9-(Methylsulfinyl)-9*H*-fluorene, *in* F-80015
2-[(5-Methylsulfinyl)-4-penten-2-ynylidene]-1,6-dioxaspiro[4.4]non-3-ene, *in* M-80175
2-(Methylsulfinyl)perimidine, *in* P-10051
2-Methyl-3-sulfolene, *in* D-70230
2-(Methylsulfonyl)adamantane, *in* A-80038
2-(Methylsulfonyl)cyclohexanone, *in* M-70025
[2-(Methylsulfonyl)ethenyl]benzene, *in* M-80170
9-(Methylsulfonyl)-9*H*-fluorene, *in* F-80015
8-(Methylsulfonyl)guanosine, *in* M-70029
1-(Methylsulfonyl)-2-phenylethylene, *in* M-80170
β-(Methylsulfonyl)styrene, *in* M-80170
(Methylsulfonyl)[(trifluoromethyl)sulfonyl]methane, M-70133
Methylsulochrin, *in* S-70083
5-*O*-Methylsulochrin, *in* S-70083
4′-*O*-Methyltectorigenin, *in* T-80112
7-*O*-Methyltectorigenin, *in* T-80112
Methylterephthalaldehyde, *see* M-60047
3-Methyl-*N*-(5*a*,6*a*,7,8-tetrahydro-4-methyl-1,5-dioxo-1*H*,5*H*-pyrrolo[1,2-*c*][1,3]oxazepin-3-yl)butanamide, M-70134
2-Methyltetrahydropyran, *see* T-60075
3-Methyltetrahydropyran, *see* T-80072
4-Methyltetrahydropyran, *see* T-80073
10-Methyl-3,3,7,7-tetrakis(trifluoromethyl)-4,5,6-benzo-1-bromo-2,8-dioxabicyclo[3.3.1]octane, *see* M-60128
4-Methyl-2,2,6,6-tetrakis(trifluoromethyl)-2*H*,6*H*-[1,2]bromoxolo[4,5,1-*hi*][1,2]benzobromoxole, M-60128
2-Methyl-6-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-1,4-benzoquinone, *see* S-60010
▷ 2-Methyl-3,4,5,6-tetranitroaniline, M-60129
▷ 3-Methyl-2,4,5,6-tetranitroaniline, M-60130
▷ 4-Methyl-2,3,5,6-tetranitroaniline, M-60131
▷ 2-Methyl-3,4,5,6-tetranitrobenzenamine, *see* M-60129
▷ 3-Methyl-2,4,5,6-tetranitrobenzenamine, *see* M-60130
▷ 4-Methyl-2,3,5,6-tetranitrobenzeneamine, *see* M-60131
▷ 1-Methyl-2,3,4,5-tetranitro-1*H*-pyrrole, *in* T-60160
3-Methyl-1,3,4-thiadiazolidine-2,5-dithione, *in* M-70031
2-Methyl-Δ^2-1,3-thiazoline, *in* T-60197
Methyl 2-thiazolin-2-yl ketone, *see* A-70041
Methyl-2-thienylcarbinol, *see* T-80178
Methyl-3-thienylcarbinol, *see* T-80179
5-[(5-Methyl-2-thienyl)methylene]-2(5*H*)-furanone, M-80161
5-(5-Methyl-2-thienyl)-2,4-pentadien-4-olide, *see* M-80161
5-(5-Methyl-2-thienyl)-2-penten-4-ynoic acid, M-80162
(Methylthio)acetaldehyde, *in* M-80017
2-(Methylthio)adamantane, *in* A-80038
2-(Methylthio)benzaldehyde, *in* M-80018
3-(Methylthio)benzaldehyde, *in* M-80019
4-(Methylthio)benzaldehyde, *in* M-80020
2-(Methylthio)benzophenone, *in* M-70020
3-(Methylthio)benzophenone, *in* M-70021
4-(Methylthio)benzophenone, *in* M-70022
3-Methyl-2*H*-thiochromene, *see* M-80051
2-Methyl-2-thiocyanatopropane, M-70135
2-(Methylthio)cyclohexanone, *in* M-70025
3-(Methylthio)cyclohexanone, *in* M-70026
4-Methylthiocyclohexanone, *in* M-70027
2-(Methylthio)cyclopentanone, M-70136
4-Methylthio-2,4-decadiene-6,8-diynoic acid, M-80163
5-Methylthio-2,4-decadiene-6,8-diynoic acid, M-80164
7-Methylthio-2,6-decadiene-4,8-diynoic acid, M-80165
7-Methylthio-2,6-decadiene-4,8-diynoic acid, M-80166
9-Methylthio-2,8-decadiene-4,6-diynoic acid, M-80167
5-Methylthio-2*Z*,4*E*,6*Z*-decatetrien-8-ynoic acid methyl ester, *in* M-80164
9-Methylthio-2,4,8-decatriene-6-yn-4-olide, *see* M-80172
5-Methylthio-2,4,8-decatrien-6-ynoic acid, M-80168
7-Methylthio-2,4,6-decatrien-8-yn-4-olide, *see* M-80171
[1-(Methylthio)ethenyl]benzene, M-80169
[2-(Methylthio)ethenyl]benzene, M-80170
9-(Methylthio)-9*H*-fluorene, *in* F-80015
8-(Methylthio)guanosine, *in* M-70029
5-(3-Methylthio-2-hexen-4-ynylidene)-2(5*H*)-furanone, M-80171
5-(5-Methylthio-4-hexen-2-ynylidene)-2(5*H*)-furanone, M-80172
2-(Methylthio)-1*H*-imidazole, *in* D-80215
2-(Methylthio)-1*H*-imidazo[4,5-*b*]pyrazine, *in* D-60247
6-(Methylthio)-5*H*-imidazo[4,5-*c*]pyridazine, *in* D-70215
▷ 6-(Methylthio)inosine, *in* T-70180
1-Methylthioisoquinoline, *in* I-60132
8-*O*-Methylthiomelin, *in* T-70181
(Methylthio)methanol, M-70138
p-Methylthio-β-methylcinnamic acid, *see* M-80179
2-[(Methylthio)methyl]pyrrolidine, *in* P-70185
5-Methylthionorvaline, *see* A-60231
(Methylthio)oxirane, M-80173
1-Methylthio-5-oxo-5-phenyl-1-penten-3-yne, *see* M-80181
6-[4-(Methylthio)-1,2,3-pentatrienyl]-2*H*-pyran-2-one, M-80174
[5-(Methylthio)-4-penten-2-ynyl]benzene, *see* M-80180
2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene, M-80175
6-(4-Methylthio-3-penten-1-ynyl)-2*H*-pyran-2-one, *in* M-80174
5-(Methylthio)pentyl isothiocyanate, *see* I-60140
2-(Methylthio)perimidine, *in* P-10051
2-Methyl-3-thiophenecarboxaldehyde, M-70139
3-Methyl-2-thiophenecarboxaldehyde, M-70140
4-Methyl-2-thiophenecarboxaldehyde, M-70141
4-Methyl-3-thiophenecarboxaldehyde, M-70142
5-Methyl-2-thiophenecarboxaldehyde, M-70143
5-Methyl-3-thiophenecarboxaldehyde, M-70144
3-Methyl-2-thiophenemethanol, M-80176
4-Methyl-2-thiophenemethanol, M-80177
5-Methyl-2-thiophenemethanol, M-80178
α-Methyl-2-thiophenemethanol, *see* T-80178
α-Methyl-3-thiophenemethanol, *see* T-80179
3-Methylthio-2-phenyl-4*H*-1-benzopyran-4-one, *in* M-60025
3-[(4-Methylthio)phenyl]-2-butenoic acid, M-80179
1-[4-(Methylthio)phenyl]ethanone, *in* M-60017
1-(Methylthio)-1-phenylethylene, *see* M-80169
1-(Methylthio)-2-phenylethylene, *see* M-80170
1-Methylthio-5-phenyl-1-penten-3-yne, M-80180
5-(Methylthio)-1-phenyl-4-penten-2-yn-1-one, M-80181
[2-(Methylthio)phenyl]phenylmethanone, *in* M-70020
[3-(Methylthio)phenyl]phenylmethanone, *in* M-70021
[4-(Methylthio)phenyl]phenylmethanone, *in* M-70022
2-(Methylthio)propanoic acid, *in* M-60027
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4-(Methylthio)-2(1*H*)-pyridinethione, *in* P-60219
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5-Methylthioquinoline, *in* Q-60004
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▷ 6-(Methylthio)-9-β-D-ribofuranosyl-9*H*-purine, *in* T-70180
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▷ *N*-Nitroso-*N*-(1-methylacetonyl)-3-methylbutylamine, *see* M-60055
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6,8-Nonadien-1-ol, N-80068
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1,3-Nonadiyne, N-80069
Nonafluoromorpholine, N-60056
Nonafluorotrimethylamine, *see* T-60406
Nonafulvalene, *see* B-70104
Nonafulvene, *see* M-60073
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1-Nonen-3-ol, N-60058
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▷ 2-Norbornanone, *see* B-70098
5-Norbornene-2,3-dicarboximido carbonochloridate, *see* C-70059
5-Norbornen-2-one, *see* B-80080
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30-Norcyclopterospermol, N-60059
30-Norcyclopterospermone, *in* N-60059
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Nordracorhodin, N-70074
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2-Norerythromycin *B*, *in* N-70076
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Norharmalan, *see* D-60209
20-Nor-8,15-isopimaradiene-7,11-dione, *in* H-80217
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Norobtusifolin, *see* T-80322
23-Nor-6-oxodemethylpristimerol, *see* D-80351
17-Nor-7-oxo-8-labden-15-oic acid, *in* H-60198
28-Nor-16-oxo-17-oleanen-3β-ol, *in* M-70011
23-Nor-6-oxopristimerol, *in* D-80351
Norpatchoulenol, N-70078
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3-Nortricyclanone, *see* T-70228
Nortropane, *see* A-70278
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Obtusadiene, O-70001
Obtusifolin/, *in* T-80322
Obtusilic acid, *in* D-80017
Obtusinin, *in* H-80189
Ochrolechic acid, *see* V-80004
Ochromycinone, O-60003
Ochromycinone methyl ether, *in* O-60003
3,11,19,27,33,34,35,36-Octaazapentacyclo[27.3.1.1^{5,9}.1^{13,17}.1^{21,25}]hexatriaconta-1(33),5(34),6,8,13,(35),14,16,21(36),22,24,29,31-dodecaene, O-80002
3,6,9,17,20,23,29,30-Octaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),11(30),12,14,25,27-hexaene, O-80003
Octabisvalene, *see* P-80020
Octachloropropane, O-80004
Octacosanal, O-80005
11,11,12,12,13,13,14,14-Octacyano-1,4:5,8-anthradiquinotetramethane, O-70002
2,4-Octadecadienoic acid, O-70003
2,4-Octadecadien-1-ol, O-60004
11,17-Octadecadien-9-ynoic acid, O-80006
Octadecahydrotriphenylene, O-70004
2-Octadecanol, O-80007
4,8,12,15-Octadecatetraenoic acid, O-80008
3-Octadecene-1,2-diol, O-60005
9-Octadecene-1,12-diol, O-60006
15-Octadecene-9,11,13-triynoic acid, O-80009
2-Octadecen-1-ol, O-60007
17-Octadecen-9-ynoic acid, O-80010
2-Octadecylicosanoic acid, O-70005
5,6,10,11,16,17,21,22-Octadehydro-7,9,18,20-tetrahydrodibenzo[*e,n*][1,10]dioxacyclooctadecin, O-70006
2,6-Octadienoic acid, O-80011
2,4-Octadien-1-ol, O-70007
N,N,N′,N′,N″,N″,N‴,N‴-Octaethylbenzo[1,2-*c*:4,5-*c′*]dipyrrole-1,3,5,7-tetramine, *see* T-70125
Octaethyltetramethyl[26]porphyrin[3.3.3.3], O-60008
2,2,3,3,5,5,6,6-Octafluoromorpholine, O-60009
Octafluoronaphthalene, O-70008
4,5,7,8,12,13,15,16-Octafluoro[2.2]paracyclophane, O-60010
▷ Octahydroazocine, O-70010
5,7,9,14,16,18,28,33-Octahydro-28,33[1,2′]benzeno-7,16[2′,3′]anthraceno-5,18[1,2′]:9,14[1″,2″]-dibenzenoheptacene, *see* T-60407
Octahydro-1*H*-2-benzopyran-1-one, O-80012
Octahydro-7*H*-1-benzopyran-7-one, O-60011
Octahydrobenzo[*b*]thiophene, O-60012
Octahydro-2*H*-1-benzothiopyran, O-80013
Octahydro-2*H*-1,3-benzoxazine, O-70011
Octahydro-2*H*-3,1-benzoxazine, O-70012
▷ 6*H*,13*H*-Octahydrobis[pyridazino[1,2-*a*:1′,2′-*d*]-*s*-tetrazine], *see* O-70013
Octahydro-1*H*,4*H*,7*H*,10*H*-cyclobuta[1,2:1,4:2,3:3,4]tetracyclopentene, *see* P-70020
2,3,4,5,6,7,8,9-Octahydro-1*H*-cyclopent[*e*]-*as*-indacene, *see* O-60021
1,4,5,8,8*a*,10,11,11*a*-Octahydrocyclopent[*d*]oxecin-2,9-dione, *see* J-80005
Octahydro-3*a*,6*a*-diazapentalene, *see* T-80077
7,8,10,11,20,21,23,24-Octahydro-5,26[1′:2′]:13,18[1″,2″]dibenzenodibenzo[*i,t*][1,4,7,12,15,18]hexaoxacyclodocosin, *see* H-70086
6,7,9,10,17,18,20,21-Octahydrodibenzo[*b,k*][1,4,7,10,13,16]hexathiacyclooctadecin, *see* D-60073
2*a*,2*b*,4*a*,4*b*,4*c*,4*d*,4*e*,4*f*-Octahydrodicyclobuta[*def,jkl*]biphenylene, *see* P-60028
Octahydrodicyclopropa[*cd,gh*]pentalene, *see* T-70022
Octahydro-5*a*,10*a*-dihydroxy-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60014
Octahydro-2,7-dihydroxy-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60013
Octahydro-5*a*,10*a*-dihydroxypyrocoll, *see* O-60014
Octahydro-2,7-dihydroxypyrocoll, *see* O-60013
Octahydro-2,7:3,6-dimethano-2*H*-1-benzopyran, *see* O-70069
1,2,3,4,5,6,7,8-Octahydro-1,4:5,8-dimethanonaphthalene, *see* T-70021
1,2,3,4,4*a*,5,6,8*a*-Octahydro-4,7-dimethyl-α-methylene-1-naphthaleneacetic acid,9CI, *see* C-70004
1,2,3,4,4*a*,5,6,7-Octahydro-4*a*,5-dimethyl-2-(1-methylethenyl)naphthalene, O-60015
▷ 6*H*,13*H*-Octahydrodipyridazino[1,2-*a*:1′,2′-*d*][1,2,4,5]tetrazine, O-70013
Octahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60016
Octahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dithione, O-70014
Octahydro-1,2,4-(epoxyethanylylidene)-5*H*-6-oxacyclobut[*cd*]indene-5,8-dione, *see* D-60467
5,6,15,16,19,20,29,30-Octahydro-2,17:3,18:7,11:10,14:21,25:24,28-hexamethenobenzocyclooctacosene, O-80014
3,5,6,6*a*,7,8,9,10-Octahydro-9-hydroxy-7,8-dimethyl-3-oxo-1*H*-naphtho[1,8*a*-*c*]furan-7-acetic acid, *see* H-70226
Octahydro-2-hydroxy-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60017
1,2,3,4,4*a*,5,6,6*a*-Octahydro-11-hydroxy-4,4,6*a*,9-tetramethyl-12*bH*-benzo[*a*]xanthene-12*b*-methanol, *see* S-60030
1,4,4*a*,5,6,7,8,8*a*-Octahydro-1-hydroxy-5,5,8*a*-trimethyl-1,2-naphthalenedicarboxaldehyde, *see* W-60001
Octahydroimidazo[4,5-*d*]imidazole, O-70015
6,7,9,10,12,13,15,16-Octahydro-1,21-methano-22*H*-dibenzo[*n,q*][1,4,7,10,13]pentaoxacyclooctadecin-22,23-dione, *see* O-80097
Octahydro-1-methyl-2*H*-3,1-benzoxazine, *in* O-70012
1,2,3,3*a*,6,7,8,8*a*-Octahydro-8*a*-methyl-3-(1-methylethyl)-8-oxo-5-azulenecarboxaldehyde, *see* O-70093
1,2,3,4,5,6,7,8-Octahydro-8-oxo-2-naphthalenecarboxylic acid, O-80015
Octahydropyridazino[1,2-*a*]pyridazine, O-80016
1,2,3,4,5,6,7,8-Octahydropyridazino[4,5-*d*]pyridazine, O-60018
Octahydropyrocoll, *see* O-60016
Octahydropyrrolo[3,4-*c*]pyrrole, O-70017
Octahydro-4*H*-quinolizin-4-one, O-60019
1,2,3,3*a*,5*a*,6,7,8-Octahydro-1,4,7,7-tetramethylcyclopenta[*c*]pentalene, *see* P-70037
1,2,3,4,5,6,7,8-Octahydro-1,4,9,9-tetramethyl-4,7-methanoazulene, *see* P-60010
Octahydro-1,2,5,6-tetrazocine, O-60020
Octahydrothianaphthene, *see* O-60012
2,3,4,5,6,7,8,9-Octahydro-1*H*-triindene, O-60021
Octahydro-3,8,8-trimethyl-6-methylene-1*H*-3*a*,7-methanozulen-1-ol, *see* B-60113
Octahydro-5,5,8*a*-trimethyl-2(1*H*)-naphthalenone, *in* D-70014
1,3*a*,4,5,5*a*,6,7,8-Octahydro-1,3*a*,6-trimethyl-8-oxocyclopenta[*c*]pentalene-2-carboxylic acid, *see* S-70081
3″,3‴,4′,4‴,5,5″,7,7″-Octahydroxy-3,8″-biflavanone, *in* G-70005
2,2′,4,4′,7,7′,8,8′-Octahydroxy-1,1′-biphenanthrene, O-80017
2′,3,4′,5,5′,6,7,8-Octahydroxyflavone, O-60022
3,3′,4′,5,5′,6,7,8-Octahydroxyflavone, O-70018
Octaleno[3,4-*c*]furan, O-70019
$\Delta^{4a(8a)}$-Octalin-2,6-dione, *see* H-70063
Δ^{3}-2-Octalone, *see* H-80062
Δ^{6}-1-Octalone, *see* H-80061
$\Delta^{9,10}$-Octal-1-one-7-carboxylic acid, *see* O-80015
1,2,3,4,5,6,7,8-Octamethylanthracene, O-80018
2,2,3,3,4,4,5,5-Octamethylcyclopentanol, O-60024
Octamethylcyclopentanone, O-60025
Octamethylcyclopentene, O-60026
2,3,7,10,15,18,22,23-Octamethyl-7,19-dimethylene-1,10,14,23-tetracosatetraene, *see* T-80152
2,6,10,14,19,23,27,31-Octamethyl-2,6,10,14,18,22,26,30-dotriacontaoctaene, *see* L-70044
2,6,10,14,19,23,27,31-Octamethyl-2,6,10,14,17,22,26,30-dotriacontraoctaen-19-ol, O-70020
1,1,2,2,3,3,4,4-Octamethyl-5-methylenecyclopentane, O-60027
1,2,2,3,3,4,4,5-Octamethyl-6-oxabicyclo[3.1.0]hexane, O-70021
N,N,N′,N′,N″,N″,N‴,N‴-Octamethylpyrrolo[3,4-*c*]pyrroleteramine, *see* T-70127
2-Octanamine, *see* O-60031
Octaphenyl[4]radialene, *see* T-70128
1,2,4-Octatriene, O-80019
1,3,5-Octatriene, O-70022
2,4,6-Octatriene, O-70023
2-(3,5,7-Octatrien-1-ynyl)thiophene, O-80020
3-Octenal, O-70024
2-Octenedial, O-80021
4-Octenedial, O-70025
4-Octene-1,8-diol, O-70026
4-Octene-1,7-diyne, O-60028
5-Octenoic acid, O-80022
2-Octen-1-ol, O-60029
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4-Octen-2-one, O-60030
5-Octen-2-one, O-70028
1-Octenylbenzene, *see* P-80106
2-Octenylbenzene, *see* P-80107
1-Octenyl bromide, *see* B-70261
1-Octenyl iodide, *see* I-70051
10-[3-(2-Octenyl)oxiranyl]-5,8-decadienoic acid, *see* E-60017
3-Octen-1-yne, O-70029
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2-Octylamine, O-60031
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11,13(18)-Oleanadiene-3,24-diol, O-80030
11,13(18)-Oleanadien-3-ol, O-70032
9(11),12-Oleanadien-3-ol, O-70031
9(11),12-Oleanadien-3-one, O-60032
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12-Oleanene-3,15-diol, O-70033
12-Oleanene-3,15-diol, O-80031
12-Oleanene-3,24-diol, O-80032
13(18)-Oleanene-2,3-diol, O-60033
18-Oleanene-3,16-diol, O-80033
12-Oleanene-3,16,21,22,23,28-hexol, O-80034
12-Oleanene-3,16,21,23,28-pentol, O-50037
12-Oleanene-3α,16α,21α,22α,28-pentol, *in* O-80036
11(12)-Oleanene-3,13,23,28-tetrol, O-70034
12-Oleanene-1,2,3,11-tetrol, O-60034

12-Oleanene-3,16,23,28-tetrol, O-60035
12-Oleanene-3,21,22,28-tetrol, O-80036
12-Oleanene-1,3,11-triol, O-60036
12-Oleanene-2,3,11-triol, O-60037
12-Oleanene-2,3,23-triol, O-80037
12-Oleanene-3,15,24-triol, O-80038
12-Oleanene-3,16,28-triol, O-60038
12-Oleanene-3,9,11-triol, O-80039
13(18)-Oleanene-3,16,28-triol, O-70035
13(18)-Oleanene-3,22,24-triol, O-80040
13(18)-Oleanen-3-ol, O-70036
18-Oleanen-3-ol, O-80041
13(18)-Oleanen-3-one, *in* O-70036
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8(26),14(27)-Onceradiene-3β,21α-diol, *see* O-80045
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α-Onocerin, *see* O-80045
α-Onocerol, O-80045
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▷ Ophiobolin, *see* O-70040
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4,10(14)-Oplopadiene-3,8,9-triol, O-70042
4,10(14)-Oplopadien-3-ol, O-80046
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2-Oxa-3-azabicyclo[2.2.2]octane, O-70051
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1-Oxa-2-azaspiro[2,5]octane, O-70052
3-Oxabenzocycloheptene, *see* T-70045
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3-Oxabicyclo[3.2.0]heptan-2-one, O-70053
7-Oxabicyclo[2.2.1]hept-2-ene, O-70054
7-Oxabicyclo[4.1.0]hept-3-ene, O-60047
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8-Oxabicyclo[4.3.0]nonan-7-one, *see* H-70061
9-Oxabicyclo[4.2.1]nona-2,4,7-triene, O-70057
9-Oxabicyclo[6.1.0]non-4-ene, O-70058
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3-Oxabicyclo[3.3.0]octan-2-one, *see* H-70054
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5-Oxabicyclo[2.1.0]pent-2-ene, O-70059
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1,2,4-Oxadiazolidine-3,5-dione, O-70060
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1,3,4-Oxadiazolo[3,2-*a*]pyridin-2(3*H*)-one, O-70063
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[1,2,5]Oxadiazolo[3,4-*b*]quinoxaline, *see* F-70051
3-Oxa-1,7-heptanediol, *see* O-60097
7-Oxa[2.2.1]hericene, *see* T-70136
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▷ Oxalodihydroxamic acid, *see* O-60048
▷ Oxalohydroxamic acid, O-60048
1,1′-Oxalylbisisatin, *see* D-70466
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1-Oxa[2.2](2,7)naphthalenophane, O-80052
2-Oxapentacyclo[11.5.3.3^{4,10}.0^{7,23}0^{16,20}]-tetracosa-1(19),4,6,8,10(22),13,15,17,20,23-decaene, *see* O-80052
1-Oxaphenalene, *see* N-70009
4-Oxapipecolic acid, *see* M-70155
10-Oxa-9-selena-1-azaanthracene, *see* B-60054
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[1,4]Oxaselenino[3,2-*b*:5,6-*b*′]dipyridine, O-70066
[1,4]Oxaselenino[3,2-*b*:5,6-*c*′]dipyridine, O-70067
[1,4]Oxaselenino[3,2-*b*:6,5-*c*′]dipyridine, O-70068
3-Oxatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane, O-70069
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[1,4]Oxathiino[3,2-*b*:5,6-*c*′]dipyridine, O-60050
[1,4]Oxathiino[3,2-*c*:5,6-*b*′]dipyridine(incorr.), *see* O-60050
2-Oxatricyclo[3.3.1.1^{3,7}]decane, O-60051
2-Oxatricyclo[4.1.0^{1,6}.0^{3,5}]heptane, O-60052
7-Oxatricyclo[4.1.1.0^{2,5}]octane, O-60053
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3-(5-Oxazolyl)pyridine, O-70074
4-(2-Oxazolyl)pyridine, O-70075
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2-Oxepanethione, O-70077
3,3-Oxetanebis(methylamine), *see* B-60140
2-Oxetanecarboxaldehyde, O-80053
3,3-Oxetanedimethanamine, *see* B-60140
3,3-Oxetanedimethanol, O-60056
2-Oxetanemethanol, O-80054
3-Oxetanemethanol, O-80055
8,14-Oxido-9-oxo-8,9-secodolast-1(15)-ene-7,8-diol, *see* C-70034
11α,12α-Oxidotaraxerol, *in* E-80044
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3-Oxindolylglyoxylic acid, *see* O-80085
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▷ Oxiranetetracarbonitrile, *see* T-80023
2-Oxiranylfuran, O-70078
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▷ 3-Oxiranyl-7-oxabicyclo[4.1.0]heptane, O-80056
2-(2-Oxo-1(2*H*)-acenaphthalenylidene)-1(2*H*)-acenaphthylenone, *see* B-80067
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10-Oxo-$\Delta^{9(10\text{-}H),a}$-anthracenemalononitrile, *see* D-60164
ent-3-Oxo-16α,17-atisanediol, *see* D-70284
7-Oxo-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, O-70079
3-Oxo-2-azabicyclo[2.1.1]hexane-1-carboxylic acid, O-80057
7-Oxo-7*H*-benz[*de*]anthracene-10-carboxylic acid, O-80064
7-Oxo-7*H*-benz[*de*]anthracene-11-carboxylic acid, O-80065
7-Oxo-7*H*-benz[*de*]anthracene-1-carboxylic acid, O-80058
7-Oxo-7*H*-benz[*de*]anthracene-2-carboxylic acid, O-80059
7-Oxo-7*H*-benz[*de*]anthracene-3-carboxylic acid, O-80060
7-Oxo-7*H*-benz[*de*]anthracene-4-carboxylic acid, O-80061
7-Oxo-7*H*-benz[*de*]anthracene-8-carboxylic acid, O-80062
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β-Oxobenzenepentanal, *see* O-80092
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1-Oxo-1*H*-2-benzopyran-3-acetic acid, O-60058
2-Oxo-2*H*-benzopyran-4-acetic acid, O-60057
4-Oxo-4*H*-1-benzopyran-3-acetic acid, O-60059
9-Oxo-1*H*,9*H*-benzopyrano[2,3-*d*]-*v*-triazole, *see* B-60043
9-Oxo-2,7-bisaboladien-15-oic acid, O-80066
9-Oxo-2-bisabolen-15-oic acid, *in* O-80066
μ-Oxobis[trifluoroacetato(phenyl)iodine], *see* O-60065
2-Oxobutanal, O-80067
4-Oxobutanenitrile, *in* O-80068
3-Oxobutanethioic acid, O-70080
▷ 4-Oxobutanoic acid, O-80068
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4-Oxo-2-butynenitrile, *in* O-80070
▷ 2-Oxo-3-butynoic acid, O-80069
4-Oxo-2-butynoic acid, O-80070
2-Oxobutyraldehyde, *see* O-80067
3-Oxobutyrolactone, *see* F-80087
3-Oxo-17-carboxy-3,18-secobarbacenic acid, O-80071
7-Oxocarnosic acid, *in* T-60337
ent-7-Oxo-3,13-clerodadiene-16,15:18,19-olide, *in* H-80143
6-Oxo-3,13-clerodadien-15-oic acid, O-70081
ent-2-Oxo-3,13-clerodadien-15-oic acid, *in* C-80142
ent-2-Oxo-3,13-clerodadien-15-oic acid, *in* H-80144
ent-7-Oxo-3-clerodene-15,16:18,19-diolide, *in* H-70117
12-Oxocurvularin, *in* C-80166
3-Oxo-24-cycloarten-21-oic acid, O-80072
3-Oxocyclobutanecarboxylic acid, O-80073
4-Oxo-1-cycloheptene-1-carboxylic acid, O-70082
2-Oxocyclohexanecarboxaldehyde, O-80074
3-Oxocyclohexanecarboxaldehyde, O-80075
4-Oxocyclohexanecarboxaldehyde, O-80076
3-Oxo-1-cyclohexene-1-carboxaldehyde, O-60060
5-Oxo-1-cyclohexene-1-carboxylic acid, O-80077

5-Oxo-2-cyclohexene-1-carboxylic acid, O-80078
6-Oxo-1-cyclohexene-1-carboxylic acid, O-80079
α-(2-Oxocyclohexyl)acetophenone, *see* P-70045
6-Oxocyclonerolidol, *in* H-60111
▷ Oxocyclopentadecane, *see* C-60219
3-Oxocyclopentaneacetic acid, O-70083
2-Oxocyclopentanecarboxylic acid, O-70084
2-Oxo-1,3-cyclopentanediglyoxylic acid, O-70085
2-Oxocyclopentanediylbisglyoxylic acid, *see* O-70085
5-Oxocyclopenta[*b*]thiophene, *see* D-70183
6-Oxocyclopenta[*b*]thiophene, *see* D-70182
4-Oxocyclopenta[*c*]thiophene, *see* D-70184
3-Oxocyclopentene, *see* C-60226
α-Oxo-3-cyclopentene-1-acetaldehyde, O-60061
3-Oxo-1-cyclopentenecarboxaldehyde, O-60062
α-Oxocyclopropaneacetic acid, *see* C-60231
5-Oxocystofuranoquinol, *in* C-70260
2-Oxodecanal, O-70087
10-Oxodecanoic acid, O-60063
9-Oxo-2-decenoic acid, O-70089
9-Oxo-4,5-dehydro-4(15)-dihydrocostic acid, *in* H-60135
2-Oxodesoxyligustrin, *in* O-70090
4-Oxo-4,5-dihydrofuro[2,3-*d*]pyridazine, *see* H-60146
7-Oxo-6,7-dihydrofuro[2,3-*d*]pyridazine, *see* H-60147
7-Oxodihydrogmelinol, O-60064
1-Oxo-3*H*-1,2-dihydropyrrolo[1,2-*a*]pyrrole, *see* D-60277
μ-Oxodiphenylbis(trifluoroacetato-*O*)diiodine, O-60065
12-Oxododecanoic acid, O-60066
5-Oxo-6,8,11,14-eicosatetraenoic acid, O-80080
11-Oxoepilupeol, *in* H-80186
2-Oxo-1(10),11(13)-eremophiladien-12,8-olide, O-80081
3-Oxo-4,11(13)-eudesmadien-12-oic acid, *in* E-70061
9-Oxo-4,11(13)-eudesmadien-12-oic acid, *in* H-60135
3-Oxo-1,4-eudesmadien-12,8β-olide, *in* Y-70001
3-Oxo-4,11(13)-eudesmadien-12,8β-olide, *in* H-60136
9-Oxo-4,11(13)-eudesmadien-12,16β-olide, *in* H-60137
3-Oxo-1,4,11(13)-eudesmatrien-12,8β-olide, *see* Y-70001
1-Oxo-7(11)-eudesmen-12,8-olide, O-60067
18-Oxoferruginol, *in* A-70005
Oxoflaccidin, *in* F-80009
3-Oxo-29-friedelanal, *in* F-80082
3-Oxo-27-friedelanoic acid, *in* T-70218
5-[5-Oxo-2(5*H*)-furanylidene]-2(5*H*)-furanone, *see* B-80094
1-Oxo-4,10(14)-germacradien-12,6α-olide, *in* O-60068
1-Oxo-4-germacren-12,6-olide, O-60068
ent-20-Oxo-16-gibberellene-7,19-dioic acid, *see* G-60019
3-Oxoglutaric acid, *see* O-60084
3-Oxo-4,11(13)-guaiadien-12,8β-olide, *see* A-70054
2-Oxo-3,10(14),11(13)-guaiatrien-12,6-olide, O-70090
9-Oxogymnomitryl acetate, *in* G-70035
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17-Oxohebemacrophyllide, *in* H-60010
4-Oxoheptanal, O-60070
4-Oxoheptanedinitrile, *in* O-60071
4-Oxoheptanedioic acid, O-60071
4-Oxo-2-heptenedioic acid, O-60072
4-Oxohexanal, O-60073
5-Oxohexanal, O-70091
4-Oxo-2-hexenoic acid, O-80082
5-Oxo-3-hexenoic acid, O-70092
5-Oxo-3-hexenoic acid, O-80083
6-Oxo-4-hexenoic acid, O-80084
1-Oxohinokiol, *in* D-60306
18-Oxo-19-hydroxynerylgeraniol, *in* H-70179
2-Oxo-4-imidazolidinecarboxylic acid, O-60074
▷ 4-Oxo-2-imidazolidinethione, *see* T-70188
2-Oxo-1*H*,3*H*-imidazo[4,5-*b*]pyridine, *see* D-60249
3-Oxoindole, *see* I-60035
2-Oxo-3-indolineglyoxylic acid, O-80085
2-(2-Oxo-3-indolinyl)acetic acid, *see* D-60259
1-Oxoisoalantolactone, *in* I-80046
9-Oxoisoalantolactone, *in* I-80046
2-Oxoisoanhydrooplopanone, *in* O-50045
1-Oxoisoanhydrooplopanone (incorr.), *in* O-50045
3-Oxoisocostic acid, *in* E-70061
5-Oxoisocystofuranoquinol, *in* C-70260
10-Oxo-6-isodaucen-14-al, O-70093
2-Oxoisopentanoic acid, *see* M-80129
7-Oxo-8(14),15-isopimaradien-18-oic acid, O-70094
23-Oxoisopristimerin III, *in* I-70083
ent-15-Oxo-16-kauren-18-oic acid, O-60075
ent-15-Oxo-16-kauren-18-oic acid, O-80086
2-Oxokolavenic acid, *in* K-60013
ent-2-Oxo-7,13-labdadien-15-al, *in* D-80328
7-Oxo-8,13-labdadien-15-oic acid, O-70095
ent-6-Oxo-7,12*E*,14-labdatrien-17,11α-olide, O-60076
6-Oxo-7-labdene-15,17-dioic acid, O-60077
12-Oxolambertianic acid, *in* L-60011
3-Oxo-8,24-lanostadien-21-oic acid, O-80087
3-Oxo-8,24-lanostadien-26-oic acid, O-70096
3-Oxo-8-lanosten-26,22-olide, *in* H-60169
6-Oxolumazine, *see* P-70134
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23-Oxomariesiic acid *A*, *in* M-70012
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α-Oxo-1-naphthaleneacetic acid, O-60078
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4-Oxo-4*H*-naphtho[2,3-*b*]pyran-3-carboxaldehyde, O-80088
4-Oxo-2-nonenal, O-70097
▷ 2-Oxonorbornane, *see* B-70098
7-Oxo-11-nordrim-8-en-12-oic acid, O-60080
5-Oxo-4-octadecanolide, *see* F-80004
4-Oxooctanal, O-60081
2-Oxo-4-oxazolidinecarboxylic acid, O-60082
4-Oxopentanal, O-60083
3-Oxopentanedioic acid, O-60084
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▷ 4-Oxo-2-pentenoic acid, O-70098
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3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid, O-80090
6-(1-Oxopentyl)-1-cyclohexene-1-carboxylic acid, *see* S-80020
3-Oxo-2-pentylcyclopentaneacetic acid, O-80091
N-(3-Oxo-3*H*-phenoxazin-2-yl)acetamide, *in* A-60237
4-Oxo-2-phenyl-4*H*-1-benzopyran-3-carboxylic acid, O-60085
4-Oxo-3-phenyl-4*H*-1-benzopyran-2-carboxylic acid, O-60086
4-Oxo-2-phenyl-4*H*-1-benzothiopyran-3-carboxylic acid, O-60087
2-Oxo-4-phenyl-2,5-dihydrofuran, *see* P-60103
(2-Oxo-2-phenylethyl)carbamic acid, O-70099
2-(2-Oxo-2-phenylethyl)cyclohexanone, *see* P-70045
3-Oxo-2-phenylindolenine, *see* P-60114
3-Oxo-5-phenylpentanal, O-80092
4-Oxo-5-phenylpentanal, O-80093
5-Oxo-5-phenylpentanal, O-80094
1-Oxo-2-phenyl-1,2,3,4-tetrahydronaphthalene, *see* D-60265
1-Oxo-3-phenyl-1,2,3,4-tetrahydronaphthalene, *see* D-60266
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6-Oxo-2-phenyl-1,4,5,6-tetrahydropyrimidine, *see* D-70250
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3-Oxo-5-phenylvaleraldehyde, *see* O-80092
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3-Oxopropanoic acid, O-60090
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18-Oxo-3-virgene, O-60095
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1,8-Oxybis(ethyleneoxyethyleneoxy)-9,10-anthracenedione, O-80097
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Pentacyclo[18.2.$2^{9,12}$.$0^{4,15}$.$0^{6,17}$]hexacosa-4,6(17),9(26),11,15,20,22,23-octaene-10,25-dione, *see* P-60008
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Pentacyclo[10.4.4.$4^{4,9}$.$0^{6,23}$.$0^{14,19}$]tetracosa-4,6,8,12,14,16,17,19,21,23-decaene, *see* A-60355
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Pentacyclo[8.4.0.$0^{2,7}$.$0^{3,12}$.$0^{6,11}$]tetradeca-4,8,13-triene, P-70021
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6-(8-Pentadecenyl)salicylic acid, *in* H-60205
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1,1'-(1,3-Pentadienylidene)bisbenzene, *see* D-70489
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2-(1,3-Pentadiynyl)-5-(3,4-diacetoxy-1-butynyl)thiophene, *in* P-80025
4-[5-(1,3-Pentadiynyl)-2-thienyl]-3-butyne-1,2-diol, *in* P-80025
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4,4′,5,5′,8-Pentahydroxy-7,7′-dimethyl-[1,1′-bianthracene]-9,9′,10,10′-tetrone, *see* R-80011
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6,7,8,14,15-Pentahydroxy-11,13(16)-labdadiene, *see* L-70008
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(−)-8-Phenylmenthol, *in* M-60090
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Tetradecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenedipentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalen-1(2*H*)-amine, *see* A-80071
Tetradecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]-diylidenedipentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene-1(2*H*)-carboxaldehyde, *see* D-80521
Tetradecahydro-5,2,1,6,3,4-[2,3]butanediyl[1,4]diylidenepentaleno[2,1,6-*cde*:2′,1′,6′-*gha*]pentalene-1(2*H*)-methanol, *see* H-80201
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5-(1-Tetradecenyl)-1,3-benzodioxole, *see* M-60077
1-Tetradecylcyclopropanecarboxylic acid, T-60040
7-Tetradecyn-1-ol, T-60042
5,6,9,10-Tetradehydro-1,4:3,14-diepoxy-4-hydroxy-4,5-secofuranoeremophilane, T-80046
9,10,23,24-Tetradehydro-5,8:11,14:19,22:25,28-tetraethenodibenzo[*a,m*]cyclotetracosene, *see* T-70012
1,3,5,7-Tetraethenyladamantane, *see* T-70154
1,2,4,5-Tetraethenylbenzene, *see* T-80162
1,3,5,7-Tetraethenyltricyclo[3.3.1.1^{3,7}]decane, *see* T-70154
1,1,4,4-Tetraethoxy-2-butyne, *in* B-60351
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1,3,5,7-Tetraethynyladamantane, T-70025
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1,3,5,7-Tetraethynyltricyclo[3.3.1.1^{3,7}]decane, *see* T-70025
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2,3,4,6-Tetrafluorobenzaldehyde, T-70027
2,3,5,6-Tetrafluorobenzaldehyde, T-70028
2,3,5,6-Tetrafluoro-1,4-benzenedicarboxylic acid, T-70029
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3,4,5,6-Tetrafluoro-1,2-benzenedicarboxylic acid, T-70031
2,3,4,5-Tetrafluorobenzoic acid, T-70032
2,3,4,6-Tetrafluorobenzoic acid, T-70033
2,3,5,6-Tetrafluorobenzoic acid, T-70034
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3,3,4,4-Tetrafluorocyclobutene, T-60043
3,3,4,4-Tetrafluorodihydro-2,5-furandione, *in* T-80049
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1,2,3,5-Tetrafluoro-4,6-diiodobenzene, T-60045
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1,1,2,2-Tetrafluoro-1,2-diiodoethane, T-80050
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2,2,4,4-Tetrafluoro-1,3-dithietane, T-60048
▷ 1,1,2,2-Tetrafluoroethane, T-80051
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4,5,6,7-Tetrafluoro-1,3-isobenzofurandione, *in* T-70031
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2,3,5,6-Tetrafluoro-4-pyridinamine, *see* A-60257
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5,6,15,16-Tetrafluorotricyclo[8.2.2.2^{4,7}]hexadeca-4,6,10,12,13,15-hexaene, *see* T-60050
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1,3,4,10-Tetrahydro-9(2*H*)-acridinone, T-60052
1,2,3,4-Tetrahydroacridone, *see* T-60052
1,2,3,4-Tetrahydroanthracene, T-60053
1,2,3,4-Tetrahydro-9,10-anthracenedione, *see* T-60054
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1,2,3,4-Tetrahydroanthraquinone, T-60054
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1,2,3,4-Tetrahydrobenz[*g*]isoquinoline, T-80054
4,5,6,7-Tetrahydro-1,2-benzisoxazol-3-ol, *see* T-70037
4,5,6,7-Tetrahydro-2,1-benzisoxazol-3(3*aH*)-one, *see* T-70038
4,5,6,7-Tetrahydro-1,2-benzisoxazol-3(2*H*)-one, T-70037
4,5,6,7-Tetrahydro-2,1-benzisoxazol-3(1*H*)-one, T-70038
2,3,8,9-Tetrahydrobenzo[1,2-*b*:3,4-*b*′]bis[1,4]dithiin, T-70039
2,3,8,9-Tetrahydrobenzo[2,1-*b*:3,4-*b*′]bis[1,4]oxathiin, T-70040
7,8,8*a*,9*a*-Tetrahydrobenzo[10,11]chryseno[3,4-*b*]oxirene-7,8-diol, T-70041
6,7,8,9-Tetrahydro-5*H*-benzocycloheptene-6-carboxaldehyde, T-60055
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1,2,3,4-Tetrahydro-7*H*-benzocyclohepten-7-one, T-60057
1,3,4,5-Tetrahydro-2*H*-1,3-benzodiazepin-2-one, T-60058
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5*a*,6,11*a*,12-Tetrahydro[1,4]benzoxazino[3,2-*b*][1,4]benzoxazine, T-60059
1,2,4,5-Tetrahydro-3-benzoxepin, T-70043
1,3,4,5-Tetrahydro-2-benzoxepin, T-70044
2,3,4,5-Tetrahydro-1-benzoxepin, T-70045
1,1′,3,3′-Tetrahydro-[1,1′-bi-2*H*-indene]-2,2′-dione, *see* B-80095
2,2′,3,3′-Tetrahydro-[2,2′-bi-1*H*-indene]-1,1′-dione, *see* B-80096
4*a*,4*b*,8*a*,8*b*-Tetrahydrobiphenylene, T-60060
Tetrahydro-2,5-bis(4-hydroxy-3-methoxyphenyl)-3,4-dimethylfuran, *see* M-70003
Tetrahydrobis(4-hydroxyphenyl)-3,4-dimethylfuran, T-60061
Tetrahydro-3,4-bis(methylene)furan, T-70046
3,4,5,6-Tetrahydro-4,5-bis(methylene)pyridazine, T-60062
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1,2,3,4-Tetrahydro-9*H*-carbazol-3-amine, *see* A-60259
1,2,3,9-Tetrahydro-4*H*-carbazol-4-one, *see* O-70106
1,2,4,9-Tetrahydro-3*H*-carbazol-3-one, *see* O-70105
1,3,4,9-Tetrahydro-2*H*-carbazol-2-one, *see* O-70104
2,3,4,9-Tetrahydro-1*H*-carbazol-1-one, *see* O-70103
4*a*,5,6,7-Tetrahydrochroman-7-one, *see* H-60045
5*a*,5*b*,11*a*,11*b*-Tetrahydrocyclobuta[1,2-*b*:4,3-*b*′]benzothiopyran-11,12-dione, T-60063
1,2,3,8-Tetrahydrocyclobuta[*b*]quinoxaline-1,2-dione, *see* D-70178
7,8,9,10-Tetrahydro-6*H*-cyclohepta[*b*]naphthalene, T-70047
1,4,5,6-Tetrahydrocyclopentapyrazole, T-80055
3,3*a*,4,6*a*-Tetrahydrocyclopenta[*b*]pyrrol-2(1*H*)-one, T-70048
1,2,3,4-Tetrahydrocyclopent[*b*]indole, T-70049
4,5,6,7-Tetrahydro-1*H*-cyclopropa[*a*]naphthalene, T-70051
3,4,5,6-Tetrahydro-1*H*-cyclopropa[*b*]naphthalene, T-70050
1,4,5,6-Tetrahydrocycloprop[*e*]indene, T-70053
1,3,4,5-Tetrahydrocycloprop[*f*]indene, T-70052
1,3,4,5-Tetrahydrocycloprop[*f*]indene, T-80056
1*a*,6*b*,7*a*,12*b*-Tetrahydrodibenz[3,4:7,8]anthra[1,2-*b*:5,6-*b*′]bisoxirene, *see* D-70151
5,6,7,12-Tetrahydrodibenz[*b,e*]azocine, T-70055
5,6,11,12-Tetrahydrodibenz[*b,f*]azocine, T-70057
5,6,7,12-Tetrahydrodibenz[*b,g*]azocine, T-70056
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4*b*,8*b*,8*c*,8*d*-Tetrahydrodibenzo[*a,f*]cyclopropa[*cd*]pentalene, T-80057
4*b*,8*b*,12*b*,16*b*-Tetrahydrodibenzo[*a,f*]dibenzo[2,3:4,5]pentaleno[1,6-*cd*]pentalene, *see* T-60019
5,7,12,14-Tetrahydrodibenzo[*c,h*][1,6]dithiecin, T-80058
4*b*,8*b*,12*b*,12*d*-Tetrahydrodibenzo[2,3:4,5]pentaleno[1,6-*ab*]indene, *see* T-80215
6,7,14,15-Tetrahydrodibenzo[*b,h*][1,4,7,10]tetraoxacyclododecin, T-80059
5,6,20,21-Tetrahydro-2,16;3,10-diethano-15,11-metheno-11*H*-tribenzo[*a,e,i*]pentadecene, T-80060
4*b*,8*b*,13,14-Tetrahydrodiindeno[1,2-*a*:2′,1′-*b*]indene, T-70058
1,4,5,8-Tetrahydro-1,4:5,8-dimethanonaphthalene, *see* T-60032
3,3*a*,4,5-Tetrahydro-5,7-dimethoxy-2-methyl-3*a*-(2-propenyl)-3-(3,4,5-trimethoxyphenyl)-6(2*H*)-benzofuranone, *see* C-70175
5,6,7,7*a*-Tetrahydro-4,7-dimethylcyclopenta[*c*]pyran-1(4*aH*)-one, *see* N-60020
3,4,5,6-Tetrahydro-4,5-dimethylenepyridazine, *see* T-60062
4,4′-(Tetrahydro-3,4-dimethyl-2,5-furandiyl)bis[2-methoxyphenol], *see* M-70003
4,4′-(Tetrahydro-3,4-dimethyl-2,5-furandiyl)bisphenol, *see* T-60061
Tetrahydro-4,5-dimethyl-2-furanone, *see* D-80191
5,7,8,10-Tetrahydro-3,8-dimethyl-7,10-methanofuro[2,3-*i*][2,5]benzodioxocin-8-ol, *see* T-80046
Tetrahydro-3,4-dimethyl-6-(1-methylbutyl)-2*H*-pyran-2-one, *see* I-60038
5,6,7,8-Tetrahydro-3,8-dimethyl-5-(1-methylethyl)-1,2-naphthalenedione, *see* M-80006
Tetrahydro-2,2-dimethyl-5-(1-methyl-1-propenyl)furan, T-80061
Tetrahydro-5,6-dimethyl-2*H*-pyran-2-one, T-70059
1,2,3,4-Tetrahydro-2,4-dioxopyrido[2,3-*d*]pyrimidine, *see* P-60236
1,2,3,4-Tetrahydro-2,4-dioxopyrido[3,4-*d*]pyrimidine, *see* P-60237
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidineacetic acid, T-70060
1,2,3,4-Tetrahydro-2,4-dioxo-5-pyrimidinecarboxaldehyde, T-60064
Tetrahydrodiphenospiropyran, *see* T-70094
5,6,12,13-Tetrahydro-1,17-(ethano[1,3]benzenoethano)-7,11:18,22-dimethenodibenzo[*a,h*]cyclooctadecene, T-80062

5,6,11,12-Tetrahydro-1,10-ethanodibenzo[*a,e*]cyclooctene, *see* C-60228
Tetrahydro-4*a*,8*a*-ethanonaphthalene-1,5(2*H*,6*H*)-dione, *see* T-60261
7,8,9,10-Tetrahydrofluoranthene, T-70061
Tetrahydro-3,4-furandiamine, T-70062
Tetrahydro-3-furanthiol, T-80063
4-(Tetrahydro-2-furanyl)morpholine, T-60065
5,6,7,8-Tetrahydro-4,4′,5,6,6′,7,8-heptahydroxy-2,2′-dimethoxy-7,7′-dimethyl-1,1′-bianthracene-9,9′,10,10′-tetrone, *see* A-60079
2,2′,3,3′-Tetrahydro-5,5′,6,6′,8,8′-hexahydroxy-2,2′-dimethyl[9,9′-bi-4*H*-naphtho[2,3-*b*]pyran]-4,4′-dione, *see* C-60029
5,6,11,12-Tetrahydro-5,6,11,12,13,20-hexamethyl-5*a*,11*a*-(imino[1,2]benzenimino)quinoxalino[2,3-*b*]quinoxaline, T-80064
3,3*a*,7,7*a*-Tetrahydro-3-hydroxy-3,6-dimethyl-2-(3-methyl-2-butenylidene)-4(2*H*)-benzofuranone, *see* B-60138
5,6,7,8-Tetrahydro-3-hydroxy-2-(2-hydroxy-1-methylethyl)-8,8-dimethyl-1,4-phenanthrenedione, *see* N-60017
1,2,3,4-Tetrahydro-4-hydroxyisoquinoline, T-60066
1,2,3,4-Tetrahydro-5-hydroxyisoquinoline, T-80065
1,2,3,4-Tetrahydro-7-hydroxyisoquinoline, T-80066
Tetrahydro-2-(4-hydroxy-3-methoxyphenyl)-4-[(4-hydroxy-3-methoxyphenyl)methyl]-3-furanmethanol, *see* L-70019
3,4,7,8-Tetrahydro-11-(2-hydroxy-4-methoxyphenyl)-2,2,6,6-tetramethyl-2*H*,6*H*,12*H*-benzo[1,2-*b*;3,4-*b*′;5,6-*b*″]tripyran-12-one, T-80067
▷ 1-(Tetrahydro-5-hydroxy-4-methyl-3-furanyl)ethanone, *see* B-60194
3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2*H*-pyran-2-one, T-60067
Tetrahydro-3-hydroxy-4-methyl-2*H*-pyran-2-one, *in* D-60353
1,2,3,4-Tetrahydro-3-(hydroxymethyl)-1-(3,4,5-trimethoxyphenyl)-2-naphthalenecarboxylic acid lactone, *see* T-80080
1,2,3,4-Tetrahydro-1-hydroxy-2-naphthalenecarboxylic acid, T-70063
1,2,3,4-Tetrahydro-1-hydroxy-2-naphthalenemethanol, T-70064
1,2,3,4-Tetrahydro-1-hydroxy-2-naphthoic acid, *see* T-70063
Tetrahydro-2-(4-hydroxyphenyl)-5-(4-hydroxy-3-methoxyphenyl)-3,4-dimethylfuran, *in* T-60061
1,2,3,6-Tetrahydro-3-hydroxypicolinic acid, *see* T-60068
Tetrahydro-5-(2-hydroxypropyl)-α-methyl-2-furanacetic acid, *see* N-70069
1,2,3,6-Tetrahydro-3-hydroxy-2-pyridinecarboxylic acid, T-60068
1,2,5,6-Tetrahydro-5-hydroxy-3-pyridinecarboxylic acid, T-70065
1,2,5,6-Tetrahydro-4-hydroxypyrimidine, *see* T-60089
▷ Tetrahydro-4-hydroxy-*N,N,N*,5-tetramethyl-2-furanmethanaminium, *see* M-60153
Tetrahydroimidazo[4,5-*d*]imidazole-2,5(1*H*,3*H*)-dione, T-70066
2,3,6,7-Tetrahydro-*as*-indacene-1,8-dione, T-70069
2,3,5,6-Tetrahydro-*s*-indacene-1,7-dione, T-70067
2,3,6,7-Tetrahydro-*s*-indacene-1,5-dione, T-70068
3,5,6,7-Tetrahydro-4*H*-inden-4-one, T-70070
1,5,6,8*a*-Tetrahydro-3(2*H*)-indolizinone, T-70071
5,6,7,8-Tetrahydro-2(3*H*)-indolizinone, T-80068
2,3,5,6,7,8-Tetrahydroindolizin-2-one, *see* T-80068
Tetrahydroindoxazen-3-one, *see* T-70037
Tetrahydro-2-iodofuran, T-80069
Tetrahydro-3-iodo-2*H*-pyran-2-one, T-60069
3*a*,4,7,7*a*-Tetrahydro-1(3*H*)-isobenzofuranone, T-70072
3*a*,4,7,7*a*-Tetrahydro-1*H*-isoindole-1,3(2*H*)-dione, T-80070
1,2,3,4-Tetrahydro-1-isoquinolinecarboxylic acid, T-60070
Tetrahydroisoquinolinedione, *see* D-80217
1,2,3,4-Tetrahydro-4-isoquinolinol, *see* T-60066
1,2,3,4-Tetrahydro-7-isoquinolinol, *see* T-80066
4,5,6,7-Tetrahydroisoxazolo[4,5-*c*]pyridin-3-ol, T-60071
4,5,6,7-Tetrahydroisoxazolo[5,4-*c*]pyridin-3-ol, T-60072
4,5,6,7-Tetrahydroisoxazolo[4,5-*c*]pyridin-3(2*H*)-one, *see* T-60071
4,5,6,7-Tetrahydroisoxazolo[5,4-*c*]pyridin-3(2*H*)-one, *see* T-60072
1,2,3,4-Tetrahydro-7-methoxyisoquinoline, *in* T-80066
4,5,6,7-Tetrahydro-3-methoxyisoxazolo[4,5-*c*]pyridine, *in* T-60071
4-[2-[Tetrahydro-6-(4-methoxyphenyl)-2*H*-pyran-2-yl]ethyl]phenol, *see* C-80032
N-(5*a*,6,7,8-Tetrahydro-4-methyl-1,5-dioxo-1*H*,5*H*-pyrrolo[1,2-*c*][1,3]oxazepin-3-yl)hexanamide, *in* M-70134
4,5,6,7-Tetrahydro-1-methylene-1*H*-indene, T-70073
1,2,3,4-Tetrahydro-1-methylenenaphthalene, T-60073
Tetrahydro-4-methylene-5-oxo-2-pentyl-3-furancarboxylic acid, *see* M-70079
Tetrahydro-6-methylene-2*H*-pyran-2-one, T-70074
1,2,3,4-Tetrahydro-3-methyl-3-isoquinolinecarboxylic acid, T-60074
Tetrahydro-6-methyl-3-methylene-6-(4-oxopentyl)-2,5-(3*H*,4*H*)-benzofurandione, *see* U-60001
7,8,9,9*a*-Tetrahydro-3-[(3-methyl-1-oxobutyl)amino]-4-methyl-1*H*,5*H*-pyrrolo[1,2-*c*][1,3]oxazepine-1,5-dione, *see* M-70134
Tetrahydro-4-methyl-5-oxo-2-pentyl-3-furancarboxylic acid, *see* P-60067
1,2,3,4-Tetrahydro-6-methyl-2-oxopyridine, *see* D-80229
Tetrahydro-4-methyl-5-pentyl-2-furanone, *see* D-80227
▷ 1,2,3,6-Tetrahydro-1-methyl-4-phenylpyridine, *in* T-60081
3,4,5,6-Tetrahydro-6-(2-methyl-1-propenyl)-1*H*-azepino[5,4,3-*cd*]indole, *see* A-60316
Tetrahydro-2-methylpyran, T-60075
Tetrahydro-3-methyl-2*H*-pyran, T-80072
Tetrahydro-4-methyl-2*H*-pyran, T-80073
Tetrahydro-4-methyl-2*H*-pyran-2-one, *in* H-70182
(Tetrahydro-4-methyl-2*H*-pyran-2-yl)-2-propanone, T-80074
Tetrahydro-2-(4-morpholinyl)furan, *see* T-60065
3,4,7,8-Tetrahydro-2,6(1*H*,5*H*)-naphthalenedione, *see* H-70063
5,6,7,8-Tetrahydro-1,4-naphthalenedione, *see* T-80076
3,4,5,6-Tetrahydro-1(2*H*)-naphthalenone, T-80075
1-(1,2,3,4-Tetrahydro-2-naphthalenyl)ethanone, *see* A-70053
5,6,7,8-Tetrahydro-1,4-naphthoquinone, T-80076
1,1′-(1,2,3,4-Tetrahydronaphthylidene), *see* B-70165
3,6,7,8-Tetrahydro-2*H*-oxocin, T-60076
2,3,4,5-Tetrahydro-2-oxo-1,5-ethanobenzazepine, *see* D-60239
N-(Tetrahydro-2-oxo-3-furanyl)hexadecanamide, *in* A-60138
▷ Tetrahydro-2-oxoglyoxaline, *see* I-70005
7,8,9,9*a*-Tetrahydro-3-[(1-oxohexyl)amino]-4-methyl-1*H*,5*H*-pyrrolo[1,2-*c*][1,3]oxazepine-1,5-dione, *in* M-70134
1,2,5,6-Tetrahydro-4-oxopyrimidine, *see* T-60089
1,2,3,4-Tetrahydro-2-oxo-4-quinolinecarboxylic acid, T-60077
1,2,3,4-Tetrahydro-4-oxo-6-quinolinecarboxylic acid, T-60078
1,2,3,4-Tetrahydro-4-oxo-7-quinolinecarboxylic acid, T-60079
2,2′,3,3′-Tetrahydro-3′,5,5′,7,7′-pentahydroxy-2,2′-bis(4-hydroxyphenyl)[3,8′-bi-4*H*-1-benzopyran]-4,4′-dione, *see* G-70005
5,6,6*a*,6*b*-Tetrahydro-3,5,6,6*b*,10-pentahydroxy-4,9-perylenedione, *see* A-80051
1,2,3,4-Tetrahydropentalene, T-70076
1,2,3,5-Tetrahydropentalene, T-70077
1,2,4,5-Tetrahydropentalene, T-70078
1,2,3,3*a*-Tetrahydropentalene, T-70075
1,2,4,6*a*-Tetrahydropentalene, T-70079
1,2,6,6*a*-Tetrahydropentalene, T-70080
1,3*a*,4,6*a*-Tetrahydropentalene, T-70081
1,3*a*,6,6*a*-Tetrahydropentalene, T-70082
3,3*a*,6,6*a*-Tetrahydro-1(2*H*)-pentalenone, T-70083
4,5,6,6*a*-Tetrahydro-2(1*H*)-pentalenone, T-70084
6,7,8,9-Tetrahydro-6-phenyl-5*H*-benzocyclohepten-5-one, T-60080
1,2,3,6-Tetrahydro-4-phenylpyridine, T-60081
Tetrahydro-2-phenyl-2*H*-1,2-thiazin-3-one, *in* T-60095
Tetrahydro-3-(phenythio)furan, *in* T-80063
Δ^4-Tetrahydrophthalide, *see* T-70072
1,2,3,6-Tetrahydrophthalimide, *see* T-80070
Tetrahydro-2-(2-piperidinyl)furan, T-60082
Tetrahydropiperinic acid, *see* M-80085
Tetrahydro-1*H*,5*H*-4,7*a*-propanopyrrolizinium, *see* A-80206
Tetrahydro-2*H*-pyran-2-thione, T-70085
Tetrahydro-1*H*,5*H*-pyrazolo[1,2-*a*]pyrazole, T-80077
Tetrahydro-1*H*,5*H*-pyrazolo[1,2-*a*]pyrazole-1,5-dione, T-70087
Tetrahydro-1*H*-pyrazolo[1,2-*a*]pyridazine-1,3(2*H*)-dione, T-70088
4,5,9,10-Tetrahydropyrene, T-60083
3,4,8,9-Tetrahydropyrene (obsol.), *see* T-60083
3*b*,4*a*,7*b*,8*a*-Tetrahydropyreno[4,5-*b*:9,10-*b*′]bisoxirene, *see* D-70152
▷ 1,2,3,6-Tetrahydropyridine, T-70089
2,3,4,5-Tetrahydropyridine, T-70090
1,2,3,6-Tetrahydro-3-pyridinecarboxylic acid, T-60084
6,7,8,9-Tetrahydro-5*H*-pyrido[2,3-*b*]azepine, T-70091
6,7,8,9-Tetrahydro-5*H*-pyrido[3,2-*b*]azepine, T-70092
7,8,9,10-Tetrahydropyrido[1,2-*a*]azepin-4(6*H*)-one, T-60085
5,6,9,10-Tetrahydro-4*H*,8*H*-pyrido[3,2,1-*ij*][1,6]naphthyridine, T-60086
5-(3,4,5,6-Tetrahydro-3-pyridylidenemethyl)-2-furanmethanol, T-60087
Tetrahydro-2(1*H*)-pyrimidinone, T-60088
Tetrahydro-4(1*H*)-pyrimidinone, T-60089
▷ 3,4,5,6-Tetrahydro-2(1*H*)-pyrimidinone, *in* T-60088
Tetrahydro-2-(2-pyrrolidinyl)furan, T-60090
Tetrahydro-1*H*-pyrrolizin-2(3*H*)-one, T-60091
2,3,5,6-Tetrahydro-1*H*-pyrrolizin-6-one, *see* D-80250
1,2,3,4-Tetrahydroquinoline, T-70093
1,2,3,4-Tetrahydro-5-quinolinol, *see* T-80065

6,7,8,9-Tetrahydro-4*H*-quinolizin-4-one, T-60092
3,3′,4,4′-Tetrahydro-2,2′-spirobi[2*H*-1-benzopyran], T-70094
2,2′,3,3′-Tetrahydro-3′,5,7,8′-tetrahydroxy-2′,2′-dimethyl[2,6′-bi-4*H*-1-benzopyran]-4-one, *see* S-60031
5,6,8,13-Tetrahydro-1,7,9,11-tetrahydroxy-8,13-dioxo-3-(2-oxopropyl)benzo[*a*]naphthacene-2-carboxylic acid, T-70095
2,3,4,4*a*-Tetrahydro-5,6,8,10-tetrahydroxy-7-(2-hydroxy-1-methylethyl)-1,1,4*a*-trimethyl-9(1*H*)-phenanthrenone, *see* C-60157
5,6,7,8-Tetrahydro-5,7,9,10-tetrahydroxy-2-methoxy-7-methyl-1,4-anthracenedione, *see* A-60322
1,2,3,4-Tetrahydro-1,2,4,5-tetrahydroxy-7-methoxy-2-methylanthraquinone, T-80078
1,2,12*a*,12*b*-Tetrahydro-1,4,9,12*a*-tetrahydroxy-3,10-perylenedione, *see* A-60078
1,2,3,4-Tetrahydro-1,1,5,7-tetramethyl-6-(3-methylpentyl)naphthalene, *see* R-80017
Tetrahydro-1,3,4,6-tetranitroimidazo[4,5-*d*]imidazole-2,5-(1*H*,3*H*)-dione, T-70096
▷ Tetrahydro-1,2,4,5-tetrazine-3,6-dione, T-70097
Tetrahydro-1,3,5,7-tetrazocine-2,6(1*H*,3*H*)-dione, T-70098
▷ Tetrahydro-2*H*-1,3-thiazine, T-60093
Tetrahydro-2*H*-1,4-thiazine-3-carboxylic acid, *see* T-70182
Tetrahydro-2*H*-1,3-thiazine-2-thione, T-60094
Tetrahydro-2*H*-1,2-thiazin-3-one, T-60095
Tetrahydro-2*H*-1,3-thiazin-2-one, T-60096
2-(Tetrahydro-2-thienyl)pyridine, T-60097
2,3,4,5-Tetrahydrothiepino[2,3-*b*]pyridine, T-60098
Tetrahydro-2-thiophenecarboxylic acid, T-70099
Tetrahydro-2*H*-thiopyran-3-amine, *see* A-70200
1,2,3,4-Tetrahydro-2-thioxo-5*H*-1,4-benzodiazepin-5-one, T-70100
2,3,5,6-Tetrahydro-1*H*,4*H*,7*H*,11*cH*-3*a*,6*a*,11*b*-triazabenz[*de*]anthracene, T-80079
Tetrahydro-1,2,4-triazine-3,6-dione, T-60099
1,2,3,4-Tetrahydro-1,3,8-trihydroxy-6-methoxy-3-methyl-9,10-anthracenedione, *see* A-60321
5,6,7,8-Tetrahydro-6,7,8-trihydroxy-5-[[4-oxo-2-(2-phenylethyl)-4*H*-1-benzopyran-6-yl]oxy]-2-(2-phenylethyl)-4*H*-benzopyran-4-one, *see* A-70078
3*a*,4,9,9*a*-Tetrahydro-9-(3,4,5-trimethoxyphenyl)naphtho[2,3-*c*]furan-1(3*H*)one, T-80080
7,8,11,11*a*-Tetrahydro-3,6,10-trimethylcyclodeca[*b*]furan-2(4*H*)-one, *see* G-60022
Tetrahydro-α,α,5-trimethyl-2-furanmethanol, *see* P-60160
Tetrahydro-2,2,6-trimethyl-2*H*-pyran-3-ol, T-80081
1,2,3,4-Tetrahydrotriphenylene, T-80082
1,4,5,8-Tetrahydrotriphenylene, T-80083
Tetrahydro-1,6,7-tris(methylene)-1*H*,4*H*-3*a*,6*a*-propanopentalene, T-70101
6,7,12,16-Tetrahydroxy-8,12-abietadiene-11,14-dione, T-80084
2,6,7,11-Tetrahydroxy-5,7,9(11),13-abietatetraen-12-one, T-80085
2α,6α,7,11-Tetrahydroxy-7,9(11),13-abietatrien-12-one, *in* D-70282
3′,4,4′,6-Tetrahydroxyaurone, *see* A-80188
1,2,3,4-Tetrahydroxybenzene, *see* B-60014
1,3,8,9-Tetrahydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, *see* T-80087
2,3,5,6-Tetrahydroxybenzoic acid, T-60100
▷ 2,3,7,8-Tetrahydroxy[1]benzopyrano[5,4,3-*cde*][1]benzopyran-5,10-dione, *see* E-70007
3,3′,4,4′-Tetrahydroxybibenzyl, T-60101
3,3′,4,5-Tetrahydroxybibenzyl, T-60102
4,4′,5,5′-Tetrahydroxy-1,1′-binaphthyl, T-70102
4,4′,5,5′-Tetrahydroxy-1,1′-binaphthyl, T-80086
2,2′,3,4-Tetrahydroxybiphenyl, *see* B-70122
2,2′,3,4-Tetrahydroxybiphenyl, *see* B-80125
2,3,3′,4-Tetrahydroxybiphenyl, *see* B-80126
2,3,4,4′-Tetrahydroxybiphenyl, *see* B-70123
2,3,4,4′-Tetrahydroxybiphenyl, *see* B-80127
2,3′,4′,5′-Tetrahydroxybiphenyl, *see* B-80128
4,4′,5,5′-Tetrahydroxy-2,2′-bis(hydroxymethyl)-[9,9′-bianthracene]-10,10′(9*H*,9′*H*)-dione, *see* A-80049
2′,3,4,4′-Tetrahydroxychalcone, *see* D-80362
2′,3′,4,4′-Tetrahydroxychalcone, *see* H-80245
2′,4,4′,6′-Tetrahydroxychalcone, *see* H-80246
3,4,6,8-Tetrahydroxy-11,13-clerodadien-15,16-olide, T-70103
1,3,8,9-Tetrahydroxycoumestan, T-80087
2,3,8,9-Tetrahydroxycoumestan, T-80088
3,4,8,9-Tetrahydroxycoumestan, T-80089
5,7,11,12-Tetrahydroxycoumestan, *see* T-80087
(1α,3α,4α,5β)-1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid, *see* Q-70005
3,4,5,6-Tetrahydroxy-1-cyclohexene-1-methanol, *see* H-70172
2,4,6,10-Tetrahydroxy-8-daucene, *see* D-70009
1,4,6,9-Tetrahydroxydihydro-β-agarofuran, T-80090
2,4,4′,6-Tetrahydroxydihydrochalcone, *see* H-80243
2,4,4′,6-Tetrahydroxydihydrochalcone, *see* H-80244
2,4,5,6-Tetrahydroxy-9,10-dihydrophenanthrene, *see* D-70247
3′,4′,5,5′-Tetrahydroxy-6,7-dimethoxyflavone, *in* H-70081
3′,4′,5,7-Tetrahydroxy-5′,6-dimethoxyflavone, *in* H-70081
4′,5,6,7-Tetrahydroxy-3,3′-dimethoxyflavone, *in* H-80067
2,5,6,8-Tetrahydroxy-3,7-dimethoxy-1,4-naphthoquinone, *in* H-60065
2,5,7,8-Tetrahydroxy-3,6-dimethoxy-1,4-naphthoquinone, *in* H-60065
4,4′,5,5′-Tetrahydroxy-2,2′-dimethyl-[1,1′-bianthracene]-9,9′,10′,10′-tetrone, *see* S-80031
4,4′,5,5′-Tetrahydroxy-2,2′-dimethyl-1,1′-bianthraquinone, *see* S-80031
2′,4′,5,7-Tetrahydroxy-3′,8-diprenylisoflavone, *see* H-80177
5,8,10,11-Tetrahydroxy-2,6-dodecadienoic acidδ-lactone triacetate, *see* H-70236
2,3,22,23-Tetrahydroxy-6-ergostanone, *see* T-70116
2α,3α,22*R*,23*R*-Tetrahydroxy-5α-ergost-24(28)-en-6-one, *see* D-70544
3′,4′,5,7-Tetrahydroxyflavan, T-60103
2′,5,7,8-Tetrahydroxyflavanone, T-70104
3,4′,5,7-Tetrahydroxyflavanone, T-60104
3′,4′,5,7-Tetrahydroxyflavanone, T-70105
3′,4′,6,7-Tetrahydroxyflavanone, T-70106
3,5,6,7-Tetrahydroxyflavanone, T-60105
2′,3′,5,7-Tetrahydroxyflavone, T-60106
2′,5,6,6′-Tetrahydroxyflavone, T-70107
2′,5,6′,7-Tetrahydroxyflavone, T-50153
3′,4′,5,6-Tetrahydroxyflavone, T-70108
3′,4′,6,7-Tetrahydroxyflavone, T-80092
3,4′,5,7-Tetrahydroxyflavylium, T-80093
2,3,4,5-Tetrahydroxy-9*H*-fluoren-9-one, T-70109
5β,10α,14*R*,16α-Tetrahydroxy-3,6-grayanotoxanedione, *in* G-80039
3,4,8,10-Tetrahydroxy-1-guaien-12,6-olide, T-80094
7,9,11,15-Tetrahydroxy-2-hexacosen-1,5-olide, *in* D-70276
4,4′,5,5′-Tetrahydroxy-2-(hydroxymethyl)-2′-methyl-[9,9′-bianthracene]-10,10′(9*H*,9′*H*)-dione, *see* P-80005
2,3,3*a*,7*a*-Tetrahydroxy-3-hydroxy-2-phenyl-5*H*-furo[3,2-*b*]pyran-5-one, *see* A-60083
2′,3′,4′,7-Tetrahydroxyisoflavan, T-80095
2′,4′,5,7-Tetrahydroxyisoflavan, T-80096
2′,4′,5′,7-Tetrahydroxyisoflavan, T-80097
2′,4′,6,7-Tetrahydroxyisoflavan, T-80098
2′,3′,4′,7-Tetrahydroxyisoflavanone, T-80099
2′,4′,5,7-Tetrahydroxyisoflavanone, T-80100
2′,4′,5′,7-Tetrahydroxyisoflavanone, T-80101
3′,4′,6,7-Tetrahydroxyisoflavanone, T-80102
2′,3′,4′,7-Tetrahydroxyisoflavene, T-80103
2′,4′,7,8-Tetrahydroxyisoflavene, T-80104
2′,3′,4′,7-Tetrahydroxyisoflavone, T-80105
2′,4′,5,7-Tetrahydroxyisoflavone, T-80106
2′,4′,5′,7-Tetrahydroxyisoflavone, T-80107
2′,5,6,7-Tetrahydroxyisoflavone, T-60107
2′,5,6,7-Tetrahydroxyisoflavone, T-80108
2′,5,7,8-Tetrahydroxyisoflavone, T-70110
3′,4′,5,7-Tetrahydroxyisoflavone, T-80109
3′,4′,5′,7-Tetrahydroxyisoflavone, T-80110
3′,4′,6,7-Tetrahydroxyisoflavone, T-80111
3′,4′,7,8-Tetrahydroxyisoflavone, T-70112
4′,5,6,7-Tetrahydroxyisoflavone, T-80112
4′,5,7,8-Tetrahydroxyisoflavone, T-80113
4′,6,7,8-Tetrahydroxyisoflavone, T-70113
ent-1β,3α,7α,11α-Tetrahydroxy-16-kaurene-6,15-dione, T-60109
ent-3α,7β,14α,20-Tetrahydroxy-16-kauren-15-one, T-60110
ent-7β,11α,14*S*,20-Tetrahydroxy-16-kauren-15-one, T-70115
ent-1β,7β,14*S*,20-Tetrahydroxy-16-kauren-15-one, T-70114
6,7,18,15-Tetrahydroxy-11,13-labdadiene, *see* L-70009
3,7,15,22-Tetrahydroxy-8,24-lanostadien-26-oic acid, T-60111
2′,3,4,4′-Tetrahydroxy-3′-methoxychalcone, *in* D-80372
3,3′,5,7-Tetrahydroxy-4′-methoxyflavan, *in* P-70026
3′,4′,5,6-Tetrahydroxy-7-methoxyflavanone, *in* P-70028
3′,4′,5,7-Tetrahydroxy-6-methoxyflavanone, *in* P-70028
2′,3,5,8-Tetrahydroxy-7-methoxyflavone, *in* P-70029
3′,4′,5,7-Tetrahydroxy-8-methoxyisoflavone, *in* P-80045
3′,4′,5,7-Tetrahydroxy-3-methoxy-2′-prenylflavone, *see* P-60164
1,3,5,8-Tetrahydroxy-2-methyl-9,10-anthracenedione, *see* T-60113
1,3,4,5-Tetrahydroxy-2-methylanthraquinone, T-60112
1,3,5,8-Tetrahydroxy-2-methylanthraquinone, T-60113
3,5,7,8-Tetrahydroxy-6-(3-methyl-2-butenyl)-2-phenyl-4*H*-1-benzopyran-4-one, *see* P-70105
1,3,5,8-Tetrahydroxy-2-(3-methyl-2-butenyl)xanthone, T-60114
2,3,22,23-Tetrahydroxy-24-methyl-6-cholestanone, T-70116
3,5,6,7-Tetrahydroxy-8-methylflavone, T-70117
3,5,7,8-Tetrahydroxy-6-methylflavone, T-70118
2α,3α,22*R*,23*R*-Tetrahydroxy-24*S*-methyl-B-homo-7-oxa-5α-cholestan-6-one, *see* B-70178
▷ 2,16,20,25-Tetrahydroxy-9-methyl-19-norlanosta-5,23-diene-3,11,22-trione, *see* C-70203
3,5,6,7-Tetrahydroxy-8-methyl-2-phenyl-4*H*-1-benzopyran-4-one, *see* T-70117
3,5,7,8-Tetrahydroxy-6-methyl-2-phenyl-4*H*-1-benzopyran-4-one, *see* T-70118
1,4,5,7-Tetrahydroxynaphthalene, *see* N-80003
3′,4′,5,7-Tetrahydroxyneoflavone, *see* D-80356

2,3,19,23-Tetrahydroxy-12-oleanen-28-oic acid, T-70119
9,12,13,16-Tetrahydroxy-11-oxokauran-17-al, *see* P-70097
4β,14α,17β,20*R*-Tetrahydroxy-1-oxo-20*R*-witha-2,5,24-trienolide, *see* W-60010
3′,4′,5,8-Tetrahydroxypeltogynan-4-one, *see* C-70200
1,2,5,6-Tetrahydroxyphenanthrene, T-60115
1,2,5,7-Tetrahydroxyphenanthrene, T-80114
1,2,6,7-Tetrahydroxyphenanthrene, T-60117
1,3,5,6-Tetrahydroxyphenanthrene, T-60118
1,3,6,7-Tetrahydroxyphenanthrene, T-60119
2,3,4,7-Tetrahydroxyphenanthrene, T-80115
2,3,5,7-Tetrahydroxyphenanthrene, T-60120
2,3,6,7-Tetrahydroxyphenanthrene, T-60121
2,4,5,6-Tetrahydroxyphenanthrene, T-60122
3,4,5,6-Tetrahydroxyphenanthrene, T-60123
1-(2,3,4,5-Tetrahydroxyphenyl)-3-(2,4,5-trihydroxyphenyl)-1,3-propanedione, T-70120
2,3,12,16-Tetrahydroxy-4,7-pregnadien-20-one, T-60124
3,4′,5,7-Tetrahydroxy-8-prenylflavan, T-60125
3′,4′,5,7-Tetrahydroxy-5′-*C*-prenylflavanone, *see* S-70041
3′,4′,5,7-Tetrahydroxy-8-prenylflavone, T-80116
3,5,7,8-Tetrahydroxy-6-prenylflavone, *see* P-70105
2′,4′,5,7-Tetrahydroxy-3-*C*-prenylisoflavone, *see* L-80028
2′,4′,5,7-Tetrahydroxy-8-*C*-prenylisoflavone, *see* K-80010
2,3,8,9-Tetrahydroxypterocarpan, T-80117
2,3,9,10-Tetrahydroxypterocarpan, T-80118
3,4,8,9-Tetrahydroxypterocarpan, T-80119
3,6*a*,7,9-Tetrahydroxypterocarpan, T-80120
3,6*a*,8,9-Tetrahydroxypterocarpan, T-80121
3,4,8,9-Tetrahydroxypterocarpene, T-80122
3′,4′,5,7-Tetrahydroxy-6-*C*-sophorosylflavone, *in* I-80068
2,3′,4,5-Tetrahydroxystilbene, *see* H-70215
2,3′,4,5′-Tetrahydroxystilbene, *see* D-70335
3,3′,4,5′-Tetrahydroxystilbene, *see* D-80361
2,2′,7,7′-Tetrahydroxy-4,4′8,8′-tetramethoxy-1,1′-biphenanthrene, *in* O-80017
2′,4′,5,7-Tetrahydroxy-3,5′,6,8-tetramethoxyflavone, *in* O-60022
2′,5,5′,7-Tetrahydroxy-3,4′,6,8-tetramethoxyflavone, *in* O-60022
3′,5,5′,6-Tetrahydroxy-3,4′,7,8-tetramethoxyflavone, *in* O-70018
3′,5,5′,7-Tetrahydroxy-3,4′,6,8-tetramethoxyflavone, *in* O-70018
4′,5,5′,7-Tetrahydroxy-2′,3,6,8-tetramethoxyflavone, *in* O-60022
2,3,4,5-Tetrahydroxytoluene, *see* M-80050
2,3,4,6-Tetrahydroxytoluene, *see* M-80049
2,3,5,6-Tetrahydroxytoluene, *see* M-80048
α,3,4,5-Tetrahydroxytoluene, *see* H-80196
3,5,7,8-Tetrahydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* H-70021
5,6,7,8-Tetrahydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* H-80029
3′,5,5′,7-Tetrahydroxy-3,4′,8-trimethoxyflavone, *in* H-70021
2′,4′,5,7-Tetrahydroxy-3′,6,8-triprenylisoflavone, *in* E-70058
1,3,6,7-Tetrahydroxy-2,5,8-triprenylxanthone, *see* G-60003
1,2,3,19-Tetrahydroxy-12-ursen-28-oic acid, T-70121
1,2,3,19-Tetrahydroxy-12-ursen-28-oic acid, T-80123
1,3,19,23-Tetrahydroxy-12-ursen-28-oic acid, T-80124
2,3,19,23-Tetrahydroxy-12-ursen-28-oic acid, T-80125
2,3,19,24-Tetrahydroxy-12-ursen-28-oic acid, T-80126
2,3,6,19-Tetrahydroxy-12-ursen-28-oic acid, T-80127
2,3,7,19-Tetrahydroxy-12-ursen-28-oic acid, T-50183
3,6,19,23-Tetrahydroxy-12-ursen-28-oic acid, T-80129
1,2,3,4-Tetrahydroxy-9*H*-xanthen-9-one, *see* T-60126
1,2,4,5-Tetrahydroxy-9*H*-xanthen-9-one, *see* T-70122
1,3,5,8-Tetrahydroxy-9*H*-xanthen-9-one, *see* T-70123
1,3,6,8-Tetrahydroxy-9*H*-xanthen-9-one, *see* T-60127
1,2,3,4-Tetrahydroxyxanthone, T-60126
1,2,4,5-Tetrahydroxyxanthone, T-70122
1,3,5,8-Tetrahydroxyxanthone, T-70123
1,3,6,8-Tetrahydroxyxanthone, T-60127
2,3,4,7-Tetrahydroxyxanthone, T-60128
1,1,2,2-Tetraisopropylethane, *see* D-60393
Tetrakis(2-bromoethyl)methane, T-70124
1,1,2,2-Tetrakis(bromomethyl)ethane, *see* B-60144
1,3,4,6-Tetrakis(*tert*-butylthio)thieno[3,4-*c*]thiophene, *in* T-70170
Tetrakis(2-carboxyethyl)methane, *see* M-70036
1,3,5,7-Tetrakis(carboxymethyl)adamantane, *see* A-70064
1,1,2,2-Tetrakis(chloromethyl)ethane, *see* B-60148
Tetrakis(2-cyanoethyl)methane, *in* M-70036
1,3,5,7-Tetrakis(cyanomethyl)adamantane, *in* A-70064
Tetrakis(cyclohexylidene)cyclobutane, T-80130
1,3,5,7-Tetrakis(diethylamino)-2,6-diaza-*s*-indacene, *see* T-70125
1,3,5,7-Tetrakis(diethylamino)pyrrolo[3,4-*f*]isoindole, T-70125
1,2,4,5-Tetrakis(dimethylamino)benzene, *in* T-60012
1,2,4,5-Tetrakis(dimethylamino)benzene, *in* T-60013
Tetrakis(dimethylamino)-2,5-diazapentalene, *see* T-70127
5,8,14,17-Tetrakis(dimethylamino)[3.3]para-cyclophene, T-70126
1,3,4,6-Tetrakis(dimethylamino)pyrrolo[3,4-*c*]pyrrole, T-70127
2,3,4,5-Tetrakis(1,1-dimethylethoxy)-2,4-cyclopentadien-1-one, *see* T-70013
1,2,3,4-Tetrakis(1,1-dimethylethyl)-1,3-cyclobutadiene, *see* T-70014
1,3,5,7-Tetrakis(1,1-dimethylethyl)-*s*-indacene, *see* T-60025
Tetrakis(1,1-dimethylethyl)tricyclo[1.1.0^{2,4}]butane, *see* T-70015
Tetrakis(diphenylmethylene)cyclobutane, T-70128
Tetrakis(1,3-dithiol-2-ylidene)cyclopentanone, T-80131
1,3,4,6-Tetrakis(ethylthio)thieno[3,4-*b*]thiophene, *in* T-70170
1,1,2,2-Tetrakis(hydroxymethyl)ethane, *see* B-60159
1,3,4,6-Tetrakis(isopropylthio)thieno[3,4-*c*]thiophene, *in* T-70170
Tetrakis(mercaptomethyl)methane, *see* B-60164
Tetrakis(methylsulfinylmethyl)methane, *in* B-60164
2,3,5,6-Tetrakis(methylthio)-1,4-benzenediamine, *in* D-60031
Tetrakis(methylthiomethyl)methane, *in* B-60164
Tetrakis(phenylmethoxy)methane, *in* M-80037
▷ 2,2,4,4-Tetrakis(trifluoromethyl)-1,3-dithietane, T-60129
Tetrakis(trifluoromethylthio)ethene, T-80132
Tetrakis(trifluoromethylthio)methane, T-80133
5,10,15,20-Tetrakis(2,4,6-trimethylphenyl)-21*H*,23*H*-porphine, T-80134
2,3,9,10-Tetrakis(trimethylsilyl)[5]phenylene, T-60130
1,1,2,2-Tetrakis(2-triptycyl)ethene, *see* T-60169
1,3,5,7-Tetrakis[2-D_3-trishomocubanyl-1,3-butadiynyl]adamantane, T-70129
1-(1-Tetralinylidene)tetralin, *see* B-70165
2,3,5,6-Tetramercapto-*p*-phenylenediamine, *see* D-60031
Tetramercaptotetrathiafulvalene, T-70130
1,3,4,6-Tetramercaptothieno[3,4-*c*]thiophene, *see* T-70170
Tetramesitylporphyrin, *see* T-80134
1,2,3,4-Tetramethoxybenzene, *in* B-60014
2,3,5,6-Tetramethoxybenzoic acid, *in* T-60100
4,4′,8,8′-Tetramethoxy-[1,1′-biphenanthrene]-2,2′,7,7′-tetrol, *in* O-80017
2,2′,3,4-Tetramethoxybiphenyl, *in* B-70122
2,2′,3,4-Tetramethoxybiphenyl, *in* B-80125
2,3,3′,4-Tetramethoxybiphenyl, *in* B-80126
2,3,4,4′-Tetramethoxybiphenyl, *in* B-70123
2,3,4,4′-Tetramethoxybiphenyl, *in* B-80127
2′,3,4,5-Tetramethoxybiphenyl, *in* B-80128
▷ Tetramethoxyethene, T-80135
▷ Tetramethoxyethylene, *see* T-80135
2′,5,6,6′-Tetramethoxyflavone, *in* T-70107
3′,4′,5,6-Tetramethoxyflavone, *in* T-70108
3′,4′,6,7-Tetramethoxyflavone, *in* T-80092
2′,4′,5,7-Tetramethoxyisoflavanone, *in* T-80100
2′,4′,5′,7-Tetramethoxyisoflavone, *in* T-80107
2′,5,6,7-Tetramethoxyisoflavone, *in* T-60107
3′,4′,5′,7-Tetramethoxyisoflavone, *in* T-80110
3′,4′,6,7-Tetramethoxyisoflavone, *in* T-80111
1,2,3,4-Tetramethoxy-5-methylbenzene, *in* M-80050
5,5′,6,7-Tetramethoxy-3′,4′-methylenedioxyflavone, *in* H-70081
3′,4′,5,5′-Tetramethoxy-6,7-methylenedioxyisoflavone, *in* H-80071
1,1,8,8-Tetramethoxy-4-octene, *in* O-70025
1,2,5,6-Tetramethoxyphenanthrene, *in* T-60115
1,2,5,7-Tetramethoxyphenanthrene, *in* T-80114
1,2,6,7-Tetramethoxyphenanthrene, *in* T-60117
1,3,5,6-Tetramethoxyphenanthrene, *in* T-60118
1,3,6,7-Tetramethoxyphenanthrene, *in* T-60119
2,3,5,7-Tetramethoxyphenanthrene, *in* T-60120
2,3,6,7-Tetramethoxyphenanthrene, *in* T-60121
2,4,5,6-Tetramethoxyphenanthrene, *in* T-60122
3,4,5,6-Tetramethoxyphenanthrene, *in* T-60123
3,4,7,8-Tetramethoxy-2,6-phenanthrenediol, *in* H-60066
1-(2,3,4,5-Tetramethoxyphenyl)-3-(2,4,5-trimethoxyphenyl)-1,3-propanedione, *in* T-70120
4,4′,5,5′-Tetramethoxypolemannone, *in* P-60166
1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene, T-80136
1,2,3,4-Tetramethoxyxanthone, *in* T-60126
1,3,5,8-Tetramethoxyxanthone, *in* T-70123
1,3,5,7-Tetramethyl-2,4-adamantanedione, T-60131
1,3,5,7-Tetramethyladamantanone, T-60132
1,5,9,10-Tetramethylanthracene, T-80137
1,8,9,10-Tetramethylanthracene, T-80138
2,2,3,3-Tetramethylaziridine, T-80139
N,*N*,2,2-Tetramethyl-2*H*-azirin-3-amine, *see* D-60402
2,2,5,5-Tetramethylbicyclo[4.1.0]hept-1(6)-en-7-one, T-70131

3,3′,5,5′-Tetramethyl[bi-2,5-cyclohexadien-1-ylidene]-4,4′-dione, T-80140
2,2,5,5-Tetramethyl-3,4-bis(methylene)hexane, *see* D-80108
2,2,3,3-Tetramethyl-1,4-butanediol, T-80141
2,2,3,3-Tetramethyl-1,4-butanedithiol, T-80142
2,2,4,4-Tetramethyl-1,3-cyclobutanedione, T-80143
2,2,6,6-Tetramethylcyclohexanone, T-60133
3,3,6,6-Tetramethyl-4-cyclohexene-1,2-dione, T-60134
5,5,6,6-Tetramethyl-2-cyclohexene-1,4-dione, T-60135
2,2,5,5-Tetramethyl-3-cyclohexen-1-one, T-60136
3,3,6,6-Tetramethylcyclohexyne, T-70132
2,2,5,5-Tetramethylcyclopentaneselone, T-60137
2,2,5,5-Tetramethylcyclopentanone, T-60138
2,2,5,5-Tetramethyl-3-cyclopentene-1-thione, T-60139
2,2,5,5-Tetramethyl-3-cyclopenten-1-one, T-60140
2,2,3,3-Tetramethylcyclopropanecarboxaldehyde, T-70133
2,2,3,3-Tetramethylcyclopropanecarboxylic acid, T-80144
2,2,3,3-Tetramethylcyclopropanemethanol, T-70134
2,2,8,8-Tetramethyl-5,5-dihydroxy-3,4,6,7-nonanetetrone, *in* T-60148
Tetramethyldimethylenediurea, *in* T-70098
2-(3,7,11,15-Tetramethyl-5,13-dioxo-2,6,10,14-hexadecatetraenyl)-6-methylhydroquinone, *in* H-70225
3,3′,5,5′-Tetramethyl-4,4′-diphenoquinone, *see* T-80140
4,4,5,5-Tetramethyl-1,2-dithiane, T-80145
2,2,3,3-Tetramethyldithiosuccinimide, *see* T-80151
3,4,7,11-Tetramethyl-1,3,6,10-dodectetraene, T-70135
2,3,5,6-Tetramethylenebicyclo[2.2.1]heptan-7-one, T-70136
3,4-Tetramethyleneisoxazolin-5-one, *see* T-70038
4,5-Tetramethylenetetrahydro-1,3-oxazine, *see* O-70012
5,6-Tetramethylenetetrahydro-1,3-oxazine, *see* O-70011
1,1,4*a*,6-Tetramethyl-5-ethyl-6,5-oxidodecahydronaphthalene, *see* D-70533
3,7,11,15-Tetramethyl-2,6,10,13,15-hexadecapentaen-1-ol, T-70137
3,7,11,15-Tetramethyl-2-hexadecenal, *in* P-60152
3,7,11,15-Tetramethyl-2-hexadecen-1-ol, *see* P-60152
2,2,5,5-Tetramethyl-3,4-hexanedione, T-80146
2,2,5,5-Tetramethyl-3-hexenedioic acid, T-60141
1,1,3,3-Tetramethyl-2-indaneselone, T-60142
1,1,3,3-Tetramethyl-2-indanone, T-60143
1,1,3,3-Tetramethyl-2-methylenecyclohexane, T-60144
3,3,5,5-Tetramethyl-4-methylene-1-pyrazoline, *see* D-60283
7,11,15,19-Tetramethyl-3-methylene-2-(3,7,11-trimethyl-2-dodecenyl)-1-eicosanol, T-70138
2,2,3,3-Tetramethylmonothiosuccinimide, *see* D-80255
Tetramethylnaphthazarin, *see* D-60377
2′,3′,4′,5′-Tetramethyl-6′-nitroacetophenone, T-60145
2′,3′,4′,6′-Tetramethyl-5′-nitroacetophenone, T-60146
2′,3′,5′,6′-Tetramethyl-4′-nitroacetophenone, T-60147
1-(2,3,4,5-Tetramethyl-6-nitrophenyl)ethanone, *see* T-60145
1-(2,3,4,6-Tetramethyl-5-nitrophenyl)ethanone, *see* T-60146
1-(2,3,5,6-Tetramethyl-4-nitrophenyl)ethanone, *see* T-60147
2,2,8,8-Tetramethyl-3,4,5,6,7-nonanepentone, T-60148
2,5,7,7-Tetramethyloctanal, T-70139
3,3,4,4-Tetramethyl-1,2-oxathietane, T-60149
3,7,11,15-Tetramethyl-13-oxo-2,6,10,14-hexadecatetraenal, T-60150
2,2,6,6-Tetramethyl-1-oxopiperidinium (1+), T-80147
N,N,N′,N′-Tetramethyl-1,3-pentalenediamine, *see* B-80147
2,2,4,4-Tetramethyl-3-pentanol, T-80148
2,5,8,11-Tetramethylperylene, T-70140
3,4,9,10-Tetramethylperylene, T-70141
1,3,6,8-Tetramethylphenanthrene, T-60151
2,4,5,7-Tetramethylphenanthrene, T-60152
2,2,6,6-Tetramethyl-4-piperidinamine, *see* A-70201
N-(2,2,6,6-Tetramethylpiperidyl)nitrene, T-80149
2,4,6,7-Tetramethylpteridine, T-70142
3,3,5,5-Tetramethyl-4-pyrazolidinone, T-60153
3,3,5,5-Tetramethyl-4-pyrazolinethione, *see* D-60285
3,3,5,5-Tetramethyl-1-pyrazolin-4-one, *see* D-60286
3,4,5,6-Tetramethylpyridazine, T-80150
3,3,4,4-Tetramethyl-2,5-pyrrolidinedithione, T-80151
5,5,9,9-Tetramethyl-5*H*,9*H*-quino[3,2,1-*de*]acridine, T-70143
1,5,5,9-Tetramethylspiro[5.5]undeca-1,8-dien-3-one, *in* L-70025
Tetramethylsqualene, T-80152
2,4,6,8-Tetramethyl-2,4,6,8-tetraazabicyclo[3.3.0]octane, *in* O-70015
1,3,5,7-Tetramethyltetrahydro-1,3,5,7-tetrazocine-2,6(1*H*,3*H*)dione, *in* T-70098
3,3,6,8-Tetramethyl-1-tetralone, *see* D-80254
▷ 1,1,4,4-Tetramethyl-2-tetrazene, T-80153
2,2,4,4-Tetramethyl-3-thietanone, T-60154
3,3,4,4-Tetramethyl-2-thietanone, T-60155
3,3,4,4-Tetramethylthiolane, T-80154
1,3,5,7-Tetramethyltricyclo[3.3.1.1^{3,7}]decane-2,4-dione, *see* T-60131
1,3,5,7-Tetramethyltricyclo[3.3.1.1^{3,7}]decan-2-one, *see* T-60132
1,4,4,8-Tetramethyltricyclo[6.2.1.0^{2,6}]undecan-11-ol, *see* C-70032
3,4,7,11-Tetramethyl-6,10-tridecadienal, T-60156
1,3,8,8-Tetramethyl-3-[3-(trimethylammonio)propyl]-3-azoniabicyclo[3.2.1]octane, *see* T-70277
2,4,6,8-Tetramethylundecanoic acid, T-60157
▷ *p*-Tetramethylxylylene diisocyanate, *see* B-70149
Tetra(2,3-naphtho)porphin, *see* T-80155
37*H*,39*H*-Tetranaphtho-[2,3-*b*:2′,3′-*g*:2″,3″-*l*:2‴-3‴-*q*]porphine, T-80155
Tetraneurin *C*, *in* T-60158
Tetraneurin *D*, T-60158
2,3,4,6-Tetranitroacetanilide, *in* T-60159
▷ 2,3,4,6-Tetranitroaniline, T-60159
▷ 2,3,4,6-Tetranitrobenzenamine, *see* T-60159
Tetranitroglycoluril, *see* T-70096
2,3,4,5-Tetranitro-1*H*-pyrrole, T-60160
3,4,8,9-Tetraoxa-1,6-diazabicyclo[4.4.2]dodecane, T-70144
1,7,10,16-Tetraoxa-4,13-diazacyclooctadecane, T-60161
10,11,14,15-Tetraoxa-1,8-diazatricyclo[6.4.4.0^{2,7}]hexadeca-2(7),3,5-triene, T-60162
1,7,20,26-Tetraoxa-4,23-dithiacyclooctatriacontane, T-80156
21,22,23,24-Tetraoxapentacyclo[16.2.1.1^{2,5}.1^{8,11}.1^{12,15}]tetracosa-1,3,5,7,9,1,13,15,17,19-decaene, *see* T-70146
21,22,23,24-Tetraoxapentacyclo[16.2.1.1^{3,6}.1^{8,11}.1^{13,16}]tetracosa-3,5,8,10,13,15,18,20-octaene, *see* T-70147
Tetraoxaporphycene, T-70146
Tetraoxaporphyrinogen, T-70147
1,3,7,9-Tetraoxaspiro[4,5]decane, T-60163
1,4,6,10-Tetraoxaspiro[4,5]decane, T-60164
Tetraphene-7,12-quinone, *see* B-70015
Tetraphenoxyethene, T-80157
Tetraphenoxyethylene, *see* T-80157
sym-Tetraphenylacetone, *see* T-60168
2,2,4,4-Tetraphenyl-3-butenal, T-70148
1,2,3,4-Tetraphenylcyclopentadiene, T-70149
7-[(2,3,4,5-Tetraphenyl-2,4-cyclopentadien-1-ylidene)ethenylidene]-1,3,5-cycloheptatriene, *see* C-60208
1,1,1′,1′-Tetraphenyldimethylamine, T-70150
3,3,6,6-Tetraphenyl-1,4-dioxane-2,5-dione, T-60165
4,4,5,5-Tetraphenyl-1,3-dithiolane, T-60166
α,α,α′,α′-Tetraphenyldi-*p*-xylylene, *see* B-60117
Tetraphenylenefurfuran, *see* D-70471
Tetraphenylethanone, T-60167
Tetraphenylglycolide, *see* T-60165
Tetraphenylhomofulvene, *see* M-60079
1,1,5,5-Tetraphenyl-1,4-pentadien-3-one, T-80158
1,1,3,3-Tetraphenyl-2-propanone, T-60168
Tetraphenylpyrimidine, T-80159
2′,4′,5′,6′-Tetraphenyl-*m*-terphenyl, *see* H-60074
3′,4′,5′,6′-Tetraphenyl-1,1′:2′,1″-terphenyl, *see* H-60074
9,11,20,22-Tetraphenyltetrabenzo[*a,c,l,n*]pentacene-10,21-dione, T-70151
4,4,5,5-Tetraphenyltetramethylene disulfide, *see* T-60166
1,3,4,6-Tetraphenylthieno[3,4-*c*]thiophene-5-S^{IV}, T-70152
3,3,5,5-Tetraphenyl-1,2,4-trithiolane, T-70153
α,α,α′,α′-Tetraphenyl-*p*-xylylene, *see* B-60157
1,2,3,4-Tetraphenytriphenylene, T-80160
Tetraselenafulvalene, *see* B-70116
Tetratellurafulvalene, *see* B-70117
2,5,7,10-Tetrathiabicyclo[4.4.0]decane, *see* H-60051
2,5,7,9-Tetrathiabicyclo[4.3.0]non-1(6)-ene-8-thione, *see* D-80206
2,5,7,9-Tetrathiabicyclo[4.3.0]non-1(6)-en-8-one, *see* D-80205
1,4,5,8-Tetrathiadecalin, *see* H-60051
Tetrathiafulvalene, *see* B-70119
1,3,5,7-Tetrathia-*s*-indacene-2,6-dione, *see* B-70028
1,4,5,8-Tetrathianaphthalene, *see* D-70521
Tetrathioorthocarbonic acid tetrakis(trifluoromethyl) ester, *see* T-80133
Tetrathiooxalic acid, *see* E-60040
Tetrathioquadratic acid, *see* D-70364
Tetrathiosquaric acid, *see* D-70364
1-Tetratriacontanol, T-80161
Tetra(2-triptycyl)ethylene, T-60169
1,3,5,7-Tetravinyladamantane, T-70154
1,2,4,5-Tetravinylbenzene, T-80162
1,2,4,5-Tetrazine, T-60170
1,2,4,5-Tetrazine-3,6-diamine, *see* D-70045
1,2,4,5-Tetrazine-3,6-dicarboxylic acid, T-80163
1,2,4,5-Tetrazine-3,6-diol, *see* D-70268
[1,2,4,5]Tetrazino[1,6-*a*:4,3-*a′*]bis[1]azaacenaphthylene, *see* D-60076
[1,2,4,5]Tetrazino[3,4-*b*:6,1-*b′*]bisbenzothiazole, T-60171
[1,2,4,5]Tetrazino[1,6-*a*:4,3-*a′*]diisoquinoline, T-60172
[1,2,4,5]Tetrazino[1,6-*a*:4,3-*a′*]diquinoline, T-60173
1,2,4,5-Tetrazino[1,6-*a*:4,3-*a′*]diquinoxaline, *in* A-60353
▷ 1*H*-Tetrazol-5-amine, *see* A-70202
1*H*-Tetrazole-5-thiol, *in* T-60174
Tetrazole-5-thione, T-60174

2-Tetrazolin-5-one, T-60175
Tetrazolo[5,1-*a*]phthalazine, T-70155
Tetrazolo[1,5-*a*]pyrimidine, T-60176
Tetrazolo[1,5-*c*]pyrimidine, T-60177
Tetrazolo[1,5-*b*]quinoline-5,10-dione, T-70156
Tetrazolo[1,5-*b*][1,2,4]triazine, T-80164
Tetronic acid, *see* F-80087
Teuchamaedryn *A*, T-70157
Teuchamaedryn *B*, *in* T-60180
Teucjaponin *A*, *in* T-70159
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2-Thiaadamantane, *see* T-60195
2-Thiabicyclo[2.2.1]heptan-3-one, T-60186
2-Thiabicyclo[2.2.1]hept-5-ene, T-70160
2-Thiabicyclo[3.1.0]hex-3-ene, T-70161
7-Thiabicyclo[4.3.0]nonane, *see* O-60012
2-Thiabicyclo[3.3.0]octane, *see* H-60049
2-Thiabicyclo[2.2.2]octan-3-one, T-60187
7-Thiabicyclo[4.2.0]octa-1,3,5-trien-8-one, *see* B-70065
2-Thiabicyclo[2.2.2]oct-5-en-3-one, T-60188
Thiacyclonon-4-ene, *see* H-70076
1-Thia-2-cyclooctyne, T-60189
1-Thia-3-cyclooctyne, T-60190
1-Thiadecalin, *see* O-80013
13*H*-[1,3,5]Thiadiazino[3,2-*a*:5,6-*a*']bisbenzimidazole-13-thione, T-60191
1,3,4-Thiadiazole-2,5-diamine, *see* D-60049
1,2,5-Thiadiazole-3,4-dicarboxaldehyde, T-70162
▷ 1,3,4-Thiadiazolidine-2,5-dithione, *see* M-70031
[1,2,5]Thiadiazolo[3,4-*d*]pyridazine, T-70163
[1,2,5]Thiadiazolo[3,4-*d*]pyridazin-4(5*H*)-one, T-70164
2-(1,3,4-Thiadiazol-2-yl)pyridine, T-60192
4-(1,3,4-Thiadiazol-2-yl)pyridine, T-60193
1-Thiahydrindane, *see* O-60012
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1-Thianaphthalenium, *see* B-70066
2-Thianaphthalenium, *see* B-70067
3(2*H*)-Thianaphthenone, *see* B-60048
1-Thianaphthen-3-one, *see* B-60048
9*H*-10-Thia-1,4,5,9-tetraazaanthracene, *see* P-60199
1-Thia-5,8,8*b*-triazaacenaphthylene, T-80169
2-Thiatricyclo[3.3.1.1^{3,7}]decane, T-60195
3-Thiatricyclo[2.2.1.0^{2,6}]heptane, T-70165
2-Thiatricyclo[9.3.1.1^{4,8}]hexadeca-1(15),4,6,8(16),11,13-hexaene, *see* T-60194
▷ 1,3-Thiazane, *see* T-60093
1,4-Thiazane-3-carboxylic acid, *see* T-70182
1,2-Thiazan-3-one, *see* T-60095
1,4-Thiazepine, T-60196
2-Thiazolecarboxaldehyde, T-80170
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Thiazolo[4,5-*b*]pyridine, T-70166
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1-(5-Thiazolyl)ethanone, *see* A-80029
2-Thiazolyl 2-thienyl ketone, T-80174
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Thieno[2,3-*c*]cinnoline, T-60202
Thieno[3,2-*c*]cinnoline, T-60203
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3-Thienol, *see* T-60212
4*H*-Thieno[3,4-*c*]pyran-4,6(7*H*)-dione, *in* C-60018
5*H*-Thieno[2,3-*c*]pyran-5,7(4*H*)dione, *in* C-60017
Thieno[3,2-*d*]pyrimidine, T-60205
5*H*-Thieno[2,3-*c*]pyrrole, T-60206
Thieno[2',3':4,5]thieno[2,3-*c*]quinoline, T-80176
Thieno[3,4-*c*]thiophene-1,3,4,6-tetrathiol, T-70170
4*H*-Thieno[3,2-*c*]thiopyran-7(6*H*)-one, T-80177
3-(2-Thienyl)acrolein, *see* T-80184
3-(3-Thienyl)acrolein, *see* T-80185
3-(2-Thienyl)acrylic acid, *see* T-60208
▷ 2-Thienylaldehyde, *see* T-70183
1-(2-Thienyl)ethanol, T-80178
1-(3-Thienyl)ethanol, T-80179
2-(3-Thienyl)ethanol, *see* T-60211
2-[2-(2-Thienyl)ethenyl]-1*H*-pyrrole, *see* P-60250
5-(2-Thienylethynyl)-2-thiophenemethanol, T-80180
9-(2-Thienyl)-4,6-nonadien-8-yn-1-ol, T-80181
9-(2-Thienyl)-4,6-nonadien-8-yn-3-ol, *in* T-80181
9-(2-Thienyl)-6-nonen-8-yn-3-ol, *in* T-80181
8-(2-Thienyl)-1,3,5-octatriene-7-yne, *see* O-80020
5-(2-Thienyl)oxazole, T-70171
5-(2-Thienyl)-2-penten-4-ynal, T-80182
5-(2-Thienyl)-2-penten-4-ynoic acid, T-80183
3-(2-Thienyl)-2-propenal, T-80184
3-(3-Thienyl)-2-propenal, T-80185
3-(2-Thienyl)-2-propenoic acid, T-60208
3-(3-Thienyl)-2-propenoic acid, T-70172
2-Thienylpropiolic acid, *see* T-70173
3-(2-Thienyl)-2-propynoic acid, T-70173
4-[5-(2-Thienyl)-2-thienyl]-3-butyn-1-ol, *see* B-80167
Thiepano[2,3-*b*]pyridine, *see* T-60098
Thioacetoacetic acid, *see* O-70080
Thioacrylamide, *see* P-70120
2-Thiobenzpropiolactone, *see* B-70065
2,2'-Thiobisbenzoic acid, T-70174
4,4'-Thiobisbenzoic acid, T-70175
2,2'-Thiobis-1*H*-indene, *see* D-80394
2,2'-Thiobis-1*H*-isoindole-1,3(2*H*)-dione, T-70176
N,*N*'-Thiobisphthalimide, *see* T-70176
2,3'-Thiobispyridine, T-80186
2,4'-Thiobispyridine, T-80187
3,4'-Thiobispyridine, T-80188
Thiobis(trifluoromethyl)ketene, *see* B-60187
Thiocarbonic acid cyclic *O*,*O*-o-phenylene ester, *see* B-80022
1,1'-Thiocarbonyl-2,2'-pyridone, *see* C-60014
Thiochloroformic acid, *see* C-60013
1-Thiocyanatoadamantane, T-70177
3-Thiocyanato-1-propene, T-80189
▷ 2-Thiocyanato-1*H*-pyrrole, T-60209
Thiocyanic acid 1,1-dimethylethyl ester, *see* M-70135
Thiocyanic acid 2-propenyl ester, *see* T-80189
▷ Thiocyanic acid 1*H*-pyrrol-2-yl ester, *see* T-60209
Thiocyanic acid tricyclo [3.3.1.1^{3,7}]decyl ester, *see* T-70177
1-Thiocyano-1,3-butadiene, T-60210
2,2'-Thiodibenzoic acid, *see* T-70174
4,4'-Thiodibenzoic acid, *see* T-70175
Thioflavanone, *see* D-70248
1-Thioflavone, *see* P-60082
Thioflavone, *see* P-60082
Thioformaldehyde, *see* M-70037
Thiofurodysin, T-70178
Thiofurodysin acetate, *in* T-70178
Thiofurodysinin, T-70179
Thiofurodysinin acetate, *in* T-70179
1-Thio-β-D-glucopyranoside 1-[4-(methylsulfinyl)]*N*-(sulfooxy)butanimidate, *see* G-80022
▷ 2-Thiohydantoin, *see* T-70188
2-Thioimidazolidinetrione, *see* T-70187
Thioindoxyl, *see* B-60048
▷ 6-Thioinosine, T-70180
▷ Thioinosine, *see* T-70180
2-Thioisatoic anhydride, *see* D-80261
▷ Thiolactic acid, *see* M-60027
2-Thiolanecarboxylic acid, *see* T-70099
5-Thiolhistidine, *see* M-80025
Thiomandelic acid, *see* M-60024
Thiomelin, T-70181
3-Thiomorpholinecarboxylic acid, T-70182
3-Thiomorpholinone, T-80190
1-Thionianaphthalene, *see* B-70066
2-Thionianaphthalene, *see* B-70067
Thionobutyrolactone, *see* D-70210
ε-Thionocaprolactone, *see* O-70077
2-Thiono-4-oxotetrahydroquinazoline, *see* D-60296
4-Thiono-2-oxotetrahydroquinazoline, *see* D-60295
Thionophthalic anhydride, *see* T-80193
δ-Thionovalerolactone, *see* T-70085
Thioparabanic acid, *see* T-70187
Thioperoxydicarbonic dichloride, *see* B-80142
3-Thiopheneacrylic acid, *see* T-60208
3-Thiopheneacrylic acid, *see* T-70172
▷ Thiophene-2-aldehyde, *see* T-70183
▷ 2-Thiophenecarboxaldehyde, T-70183
2,5-Thiophenedimethanethiol, T-70184
2,4(3*H*,5*H*)-Thiophenedione, T-70185
3-Thiopheneethanol, T-60211
Thiophene-3-ol, T-60212
2-Thiophenesulfonic acid, T-60213
3-Thiophenesulfonic acid, T-60214
Thiophenoxtellurine, *see* P-80086
Thiophenylacetic acid, *see* B-70017
1-Thiophthalide, *see* I-70063
2*H*-Thiopyran-2,2-dicarboxylic acid, T-80191
▷ 2-Thiopyridone, *see* P-60224
▷ 4-Thiopyridone, *see* P-60225
Thiopyrrolidone, *see* P-70186
2-Thio-2,4(1*H*,3*H*)-quinazolinedione, *see* D-60296
4-Thio-2,4(1*H*,3*H*)-quinazolinedione, *see* D-60295
Thiosine, *see* A-60152
2-Thiotetrahydro-1,3-thiazine, *see* T-60094
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2-Thiothiazolone, *see* T-60200
4-Thiothymine, *see* D-70233
Thio-α-toluic acid, *see* B-70017
Thiourea *S*-trioxide, *see* A-60210
Thioxanthylium(1+), T-70186
2-Thioxobenzodioxole, *see* B-80022
3-Thioxo-1(3*H*)-benzo[*c*]thiophenone, T-80192
4-Thioxo-2-hexanone, T-60215
2-Thioxo-4,5-imidazolidinedione, T-70187
▷ 2-Thioxo-4-imidazolidinone, T-70188
3-Thioxo-1(3*H*)-isobenzofuranone, T-80193
2-Thioxo-6-phenyl-4-pyrimidinone, *see* D-60268
3-Thioxo-1,2-propadien-1-one, T-60216
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Thorectolide 25-acetate, *in* T-70189
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3-Thujene, T-80194
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Tiglic aldehyde, *in* M-80056
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6β,9α,14-Triacetoxy-1α-benzoyloxy-4β,8β-dihydroxydihydro-β-agarofuran, *in* E-60018
6β,9β,15-Triacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran, *in* P-80032
6β,9α,14-Triacetoxy-1α-benzoyloxy-4β-hydroxy-8-oxodihydro-β-agarofuran, *in* E-60018
1,1,1-Triacetoxy-1,1-dihydro-1,2-benziodoxol-3(1*H*)-one, T-60228
ent-2α,3α,6β-Triacetoxy-7α,11β-dihydroxy-16-kauren-15-one, *in* P-80047
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3α,15α,22-Triacetoxy-7α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111
3α,7α,22-Triacetoxy-15α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111
3α,15α,22*S*-Triacetoxy-7α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111
3β,15α,22*S*-Triacetoxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
3α,15α,22*S*-Triacetoxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318
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4,15,26-Triacontatriene-1,29-diyne-3,28-diol, *see* D-70550
4,15,26-Triacontatriene-1,12,18,29-tetrayne-3,14,17,28-tetrol, *see* P-70044
21-Triacontenoic acid, T-80207
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2,4,7-Triaminopteridine, T-60229
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3*H*-2,3,5-Triazabenz[*e*]indene, *see* P-60206
1,2,6-Triaza-4,5-benzindene (obsol.), *see* P-60206
1,4,7-Triazacyclododecane, T-60231
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1,2,7-Triazaindene, *see* P-70155
1,3,4-Triazaindene, *see* D-60249
▷ 1,3,5-Triazaindene, *see* I-60008
1,2,12-Triazapentacyclo[6.4.0.0^{2,17}.0^{3,7}.0^{4,11}]-dodecane, T-70205
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3,5,12-Triazatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane, T-70206
19,20,21-Triazatetracyclo[13.3.1.1^{3,7}.1^{9,13}]heneicosa-1(19),3,5,7(21),9,11,13(20),15,17-nonaene-2,8,14-trione, T-60236
▷ 1,2,4-Triazin-3-amine, *see* A-70203
1,3,5-Triazine-2,4,6-tricarboxaldehyde, T-60237
▷ 1,3,5-Triazine-2,4,6(1*H*,3*H*,5*H*)-trione, *see* C-60179
[1,3,5]Triazino[1,2-*a*:3,4-*a*′:5,6-*a*″]trisbenzimidazole, T-60238
1*H*-1,2,3-Triazole-4-carboxylic acid, T-60239
1*H*-1,2,3-Triazole-5-carboxylic acid, *in* T-60239
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1*H*-1,2,3-Triazole-4-methanamine, T-80210
1,2,4-Triazole-3(5)-sulfonic acid, T-80211
▷ *s*-Triazole-3-thiol, *see* D-60298
1*H*-1,2,4-Triazolo[3,4-*i*]purine, T-80212
1*H*-1,2,4-Triazolo[5,1-*i*]purine, T-80213
[1,2,4]Triazolo[1,5-*b*]pyridazine, T-60240
[1,2,4]Triazolo[2,3-*b*]pyridazine, *see* T-60240
[1,2,4]Triazolo[1,5-*a*]pyrimidine, T-60242
1,2,4-Triazolo[4,3-*c*]pyrimidine, T-60243
1*H*-1,2,3-Triazolo[4,5-*f*]quinoline, T-70207
1*H*-1,2,3-Triazolo[4,5-*h*]quinoline, T-70208
[1,2,4]-Triazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one, T-80214
[1,2,4]Triazolo[1,2-*a*][1,2,4]triazole-1,3,5,7(2*H*,6*H*)-tetrone, T-70209
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2′,3′,5′-Tribromoacetophenone, T-80216
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3,6,13-Tribromo-4,10:9,12-diepoxy-14-pentadecyn-7-ol, B-70195
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[(Tribromomethyl)sulfonyl]benzene, *in* T-70212
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1-(2,3,5-Tribromophenyl)ethanone, *see* T-80216
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3,4,5-Tribromo-1*H*-pyrazole, T-60246
2*a*,4*a*,6*a*-Tribromo-2*a*,4*a*,6*a*,6*b*-tetrahydrocyclopenta[*cd*]pentalene, *see* T-60248
2,3,5-Tribromothiophene, T-60247
1,5,7-Tribromo-2,6,8-trichloro-2,6-dimethyl-3-octene, T-80218
1,3,5-Tribromo-2,4,6-trifluorobenzene, T-70214
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1,3,5-Tri-*tert*-butyl-2-nitrobenzene, T-70216
2,4,6-Tri-*tert*-butylpyridine, T-70217
2,4,6-Tri-*tert*-butylpyrimidine, T-80219
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1,2,4-Trichloro-5-(2-chloroethenyl)-1,5-dimethylcyclohexane, T-80223
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2,3,4-Trichloro-2,4,6-cycloheptatrien-1-one, T-80224
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1,1,2-Trichloro-2-(diethylamino)ethylene, T-70222
1,2,2-Trichloro-*N*,*N*-diethylethanamine, *see* T-70222
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2,2,2-Trichloro-1-(3,4-dihydro-2*H*-pyan-5-yl)ethanone, *see* D-70272
▷ 1,1,1-Trichloro-3,4-epoxybutane, *see* T-60252
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2,2,2-Trichloro-1-phenylethanone, *see* T-70219
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Tricyclo[3.3.1.1^{3,7}]decane-1,3,5,7-tetraacetic acid, *see* A-70064
Tricyclo[3.3.1.1^{3,7}]decane-1,3,5,7-tetraacetonitrile, *in* A-70064
Tricyclo[3.3.1.1^{3,7}]decane-1,3,5,7-tetracarboxylic acid, *see* A-80037
Tricyclo[3.3.1.1^{3,7}]decane-2-thiol, *see* A-80038
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Tricyclo[7.3.2.0^{5,13}]dodeca-3,5,7,9,11(13)-hexaen-2-one, *see* M-70042
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Tricyclo[3.2.0.0^{2,7}]heptane, T-80240
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2,3,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, *see* T-80293
3,7,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, *see* T-80294
3,8,9-Trihydroxy-6*H*-benzofuro[3,2-*c*]benzopyran-6-one, *see* T-80295
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5,6,7-Trihydroxy-2*H*-1-benzopyran-2-one, T-80287
5,7,8-Trihydroxy-2*H*-1-benzopyran-2-one, T-80288
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3,4,5-Trihydroxybiphenyl, *see* B-80129
2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)acetophenone, T-80289
4′,5,7-Trihydroxy-3′,6-bis(3-methyl-2-butenyl)isoflavone, T-80290
▷ 3β,14β,19-Trihydroxy-5α-card-20(22)-enolide, *see* C-60168
2′,4,4′-Trihydroxychalcone, *see* D-80367
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2,3,24-Trihydroxy-13,27-cyclo-11-oleanen-28-oic acid, T-70251
2,3,24-Trihydroxy-12,27-cyclo-14-taraxeren-28-oic acid, T-70252
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3,3′,5-Trihydroxy-4′,7-dihydroxyflavan, *in* P-70026
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4′,5,7-Trihydroxy-3′,8-dimethoxyisoflavone, *in* P-80045
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1,3,8-Trihydroxy-4,7-dimethoxyxanthone, *in* P-60052
1,5,8-Trihydroxy-2,6-dimethoxyxanthone, *in* P-60052
3,4,6-Trihydroxy-1,2-dimethylcarbazole, T-70253
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6α,7β,8α-Trihydroxy-14,15-dinor-11-labden-13-one, *in* S-60052
2,3,10-Trihydroxy-6,12-dioxabenz[*a*]anthracen-7(5*H*,6*H*,12*aH*)-one, *in* C-70200
3,7,15-Trihydroxy-11,23-dioxo-8,20(22)-lanostadien-26-oic acid, T-70254
3β,7β,28-Trihydroxy-11,15-dioxo-25,26,27-trisnor-8-lanosten-24-oic acid, *see* L-60036
14α,17β,20*R*-Trihydroxy-1,4-dioxo-22*R*-witha-5,24-dienolide, *see* P-60149
2′,4,4′-Trihydroxy-3,5-di-*C*-prenylchalcone, *see* A-80010
4′,5,7-Trihydroxy-3′,5′-di-*C*-prenylflavanone, *in* A-80009
4′,5,7-Trihydroxy-3′,8-diprenylflavanone, *see* L-60021
4′,5,7-Trihydroxy-6,8-diprenylflavanone, *see* L-60030
4′,5,7-Trihydroxy-6,8-diprenylflavanone, *see* S-70034
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5,14,15-Trihydroxy-6,8,10,12,17-eicosapentaenoic acid, T-70256
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2,8,9-Trihydroxy-11-eremophilene, *see* E-70030
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5β,6β,14*R*-Trihydroxy-10(20),15-grayanotoxadien-3-one, *in* G-80040
7,9,11-Trihydroxy-2-hexacosen-1,5-olide, *see* D-70276
2,5,7-Trihydroxy-3-(5-hydroxyhexyl)-1,4-naphthoquinone, T-70262
5,6,7-Trihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80112
5,7,8-Trihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* T-80113
3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-1-benzopyrylium, *see* T-80093
2′,4′,7-Trihydroxyisoflavan, T-80302
2′,4′,7-Trihydroxyisoflavanone, T-80303
3′,4′,7-Trihydroxyisoflavanone, T-70263
4′,5,7-Trihydroxyisoflavanone, T-80304
2′,4′,7-Trihydroxyisoflavene, T-80305
2′,4′,7-Trihydroxyisoflavone, T-70264
2′,4′,7-Trihydroxyisoflavone, T-80306
2′,5,7-Trihydroxyisoflavone, T-80307
3′,4′,7-Trihydroxyisoflavone, T-80308
▷ 4′,5,7-Trihydroxyisoflavone, T-80309
4′,6,7-Trihydroxyisoflavone, T-80310
4′,7,8-Trihydroxyisoflavone, T-70265
4′,7,8-Trihydroxyisoflavone, T-80311
3′,4,5′-Trihydroxy-3-isopentadienylstilbene, *see* H-70167
ent-7β,14α,15β-Trihydroxy-1,16-kauradien-3-one, T-80312
ent-1β,3α,11α-Trihydroxy-16-kaurene-6,15-dione, T-80313
ent-1β,7β,14α-Trihydroxy-16-kaurene-3,15-dione, T-80314
ent-7β,12β,14α-Trihydroxy-16-kaurene-3,15-dione, T-80315
ent-7α,9α,15β-Trihydroxy-16-kauren-19-oic acid, T-80316
ent-3α,7β,14α-Trihydroxy-16-kauren-15-one, T-60326
ent-1β,7β,14*S*-Trihydroxy-16-kauren-15-one, T-50476
3,7,15-Trihydroxy-8,24-lanostadien-26-oic acid, T-60327
3,7,22-Trihydroxy-8,24-lanostadien-26-oic acid, T-60328
24,25,26-Trihydroxy-7,9(11)-lanostadien-3-one, *in* L-60012
3,15,22-Trihydroxy-7,9(11),24-lanostatrien-26-oic acid, T-80318
15,26,27-Trihydroxy-7,9(11),24-lanostatrien-3-one, T-60330
3,12,17-Trihydroxy-9(11)-lanosten-18,20-olide, T-70267
1,11,20-Trihydroxy-3-lupanone, T-60331
ent-14,15,19-Trihydroxymanoyl oxide, *see* E-70020
3′,4,4′-Trihydroxy-6-methoxyaurone, *in* A-80188
2′,4,4′-Trihydroxy-3-methoxychalcone, *in* D-80362
2′,4,4′-Trihydroxy-3′-methoxychalcone, *in* H-80245
5,11,12-Trihydroxy-7-methoxycoumestan, *in* T-80087
2′,4,4′-Trihydroxy-6′-methoxydihydrochalcone, *in* H-80246
2,3,10-Trihydroxy-8-methoxy-6,12-dioxabenz[*a*]anthracen-7(5*H*,6*aH*,12*aH*)-one, *in* C-70200
3,4,10-Trihydroxy-8-methoxy-6,12-dioxabenz[*a*]anthracen-7(5*H*,6*H*,12*aH*)-one, *in* C-70200
2′,5,7-Trihydroxy-4′-methoxy-6,8-diprenylflavanone, *see* L-60022
2′,4′,7-Trihydroxy-5-methoxy-3′,6-diprenylisoflavan, *see* L-60025
2′,5,8-Trihydroxy-7-methoxyflavanone, *in* T-70104
2′,5,7-Trihydroxy-6′-methoxyflavone, *in* T-50153
2′,5,7-Trihydroxy-4′-methoxyisoflavanone, *in* T-80100
4′,5,7-Trihydroxy-2′-methoxyisoflavanone, *in* T-80100
2′,3′,7-Trihydroxy-4′-methoxyisoflavene, *in* T-80103
2′,4,7-Trihydroxy-3′-methoxyisoflavene, *in* T-80103
▷ 4′,5,7-Trihydroxy-6-methoxyisoflavone, T-80319
2′,3′,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80105
2′,4′,5-Trihydroxy-7-methoxyisoflavone, *in* T-80106
2′,4′,7-Trihydroxy-5-methoxyisoflavone, *in* T-80106
2′,5,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80106
3′,4′,5-Trihydroxy-7-methoxyisoflavone, *in* T-80109
3′,5,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80109
3′,5′,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80110
3′,7,8-Trihydroxy-4′-methoxyisoflavone, *in* T-70112
4′,5,7-Trihydroxy-3′-methoxyisoflavone, *in* T-80109
4′,5,7-Trihydroxy-8-methoxyisoflavone, *in* T-80113
4′,7,8-Trihydroxy-6-methoxyisoflavone, *in* T-70113
1,3,5-Trihydroxy-4-methoxy-2-methylanthraquinone, *in* T-60112
1,3,8-Trihydroxy-5-methoxy-2-methylanthraquinone, *in* T-60113
2′,4,6′-Trihydroxy-6-methoxy-4′-methyl-2-benzophenonecarboxylic acid methyl ester, *see* S-70083
2′,4′,5-Trihydroxy-7-methoxy-6-methylisoflavanone, *see* O-80050
1,5,10-Trihydroxy-7-methoxy-3-methyl-1*H*-naphtho[2,3-*c*]pyran-6,9-dione, T-80320
3′,4′,7-Trihydroxy-5-methoxyneoflavone, *in* D-80356
1,2,4-Trihydroxy-5-methoxy-3-(8,11,14-pentadecatrienyl)benzene, *see* M-70049
4′,5,7-Trihydroxy-3′-methoxy-5′-prenylflavanone, *in* S-70041
4′,5,7-Trihydroxy-3-methoxy-6-prenylflavone, *see* T-60224
4′,6′,7-Trihydroxy-3′-methoxy-2′-prenylisoflavone, *see* K-60016
3,6a,7-Trihydroxy-9-methoxypterocarpan, *in* T-80120
3,3′,5-Trihydroxy-4′-methoxystilbene, *in* D-80361
2,3,6-Trihydroxy-4-methoxytoluene, *in* M-80049
2,3,6-Trihydroxy-5-methoxytoluene, *in* M-80048
3,4,6-Trihydroxy-2-methoxytoluene, *in* M-80049
1,3,8-Trihydroxy-5-methoxyxanthone, *in* T-70123
1,5,8-Trihydroxy-3-methoxyxanthone, *in* T-70123
2,4,5-Trihydroxy-1-methoxyxanthone, *in* T-70122
2′,4′,6′-Trihydroxy-3′-methylacetophenone, T-80321
1,2,7-Trihydroxy-6-methyl-9,10-anthracenedione, *see* T-70268
1,2,7-Trihydroxy-6-methylanthraquinone, T-70268
1,2,8-Trihydroxy-3-methylanthraquinone, T-80322
1,6,8-Trihydroxy-2-methylanthraquinone, T-70269
3,5,6-Trihydroxy-2-methylanthraquinone, *see* T-70268
3,6,8-Trihydroxy-1-methylanthraquinone-2-carboxylic acid, T-60332
3,6,8-Trihydroxy-1-methylanthraquinone-2-carboxylic acid, T-80323
1,3,8-Trihydroxy-7-methylanthraquinone (incorr.), *see* T-70269
1,6,8-Trihydroxy-3-methylbenz[*a*]anthracene-7,12-dione, T-70270
3,4,6-Trihydroxy-2-methylbenzoic acid, T-80324
3,6*a*,9-Trihydroxy-4-(3-methyl-2-butenyl)pterocarpan, *see* G-80027
1,3,6-Trihydroxy-2-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, T-80325
3α,22*R*,23*R*-Trihydroxy-24*S*-methyl-5α-cholestan-6-one, *in* T-70116
3,6*a*,7-Trihydroxy-8,9-methylenedioxypterocarpan, *in* P-80056
4′,5,7-Trihydroxy-6-methylflavone, T-80326
1,5,8-Trihydroxy-3-methyl-2-(3-methyl-2-butenyl)xanthone, *in* T-60114
2,5,8-Trihydroxy-3-methyl-6,7-methylenedioxy-1,4-naphthoquinone, T-60333
4,6,9-Trihydroxy-7-methylnaphtho[2,3-*d*]-1,3-dioxole-5,8-dione, *see* T-60333
5,6,7-Trihydroxy-18-methyloxacyclooctadec-3-en-2-one, *see* A-60312
1-(2,4,6-Trihydroxy-3-methylphenyl)ethanone, *see* T-80321
1,3,9-Trihydroxymuurolene, *see* M-80200
1,4,5-Trihydroxynaphthalene, *see* N-60005
ent-3α,10β,15β-Trihydroxy-20-norgibberellane-7,19-dioic acid 19,10-lactone, *see* G-60017
ent-6α,15,16-Trihydroxy-19-nor-4-rosen-3-one, *in* N-60061
3β,6β,19α-Trihydroxy-23-nor-4(24),12-ursadien-28-oic acid, *see* F-80014
9,12,13-Trihydroxy-10,15-octadecadienoic acid, T-80327
9,10,18-Trihydroxyoctadecanoic acid, T-60334
9*S*,12*S*,13*S*-Trihydroxy-10*E*-octadecenoic acid, *in* T-80327
4,5,6-Trihydroxyoctadec-2-en-1,17-olide, *see* A-60312
3,16,28-Trihydroxy-13(18)-oleanene, *see* O-70035
1,3,23-Trihydroxy-12-oleanen-29-oic acid, T-80328
2,3,23-Trihydroxy-12-oleanen-28-oic acid, T-70271
2,3,24-Trihydroxy-12-oleanen-28-oic acid, T-60335
2,3,24-Trihydroxy-12-oleanen-28-oic acid, T-80329
2,3,24-Trihydroxy-11,13(18)-oleonadien-28-oic acid, T-60336
5,8,9-Trihydroxy-10(14)-oplopen-3-one, T-70272
6,7,14-Trihydroxy-8(10)-oplopen-2-one (incorr.), *see* T-70272
1,3,4-Trihydroxy-6-oxabicyclo[3.2.1]octan-7-one, *in* Q-70005
7,11,12-Trihydroxy-6-oxo-8,11,13-abietatrien-20-oic acid, T-60337

3,14,15-Trihydroxy-19-oxocard-20(22)-enolide, T-80330
(3,4,5-Trihydroxy-6-oxo-1-cyclohexen-1-yl)methyl 2-butenoate, T-60338
3β,7α,15α-Trihydroxy-11-oxo-25,26,27-trisnor-8-lanosten-24-oic acid, *see* L-60037
3β,6β,19α-Trihydroxy-23-oxo-12-ursen-28-oic acid, *in* T-80129
2′,5,7-Trihydroxy-3,4′,5′,6,8-pentamethoxyflavone, *in* O-60022
3′,5,7-Trihydroxy-3,4′,5′,6,8-pentamethoxyflavone, *in* O-70018
3′,5,7-Trihydroxy-3,4′,5′,6,8-pentamethoxyflavone, *in* O-70018
4′,5,5′-Trihydroxy-2′,3,6,7,8-pentamethoxyflavone, *in* O-60022
4′,5,7-Trihydroxy-2′,3,5′,6,8-pentamethoxyflavone, *in* O-60022
4′,5,7-Trihydroxy-3,3′,5′,6,8-pentamethoxyflavone, *in* O-70018
2,3,7-Trihydroxyphenanthrene, *see* T-60339
2,4,5-Trihydroxyphenanthrene, *see* P-60071
2,4,7-Trihydroxyphenanthrene, *see* P-80080
2,3,4-Trihydroxyphenylacetic acid, T-60340
2,3,5-Trihydroxyphenylacetic acid, T-60341
2,4,5-Trihydroxyphenylacetic acid, T-60342
3,4,5-Trihydroxyphenylacetic acid, T-60343
5,6,7-Trihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, *see* T-60322
1-(2,4,6-Trihydroxyphenyl)-2-buten-1-one, T-80331
1-(2,4,6-Trihydroxyphenyl)ethanone, *see* T-70248
▷ 1-(3,4,5-Trihydroxyphenyl)ethanone, *see* T-60315
(2,4,6-Trihydroxyphenyl)phenylmethanone, *see* T-80285
1-(2,4,6-Trihydroxyphenyl)-3-phenyl-1-propanone, T-80332
3-(3,4,5-Trihydroxyphenyl)propanal, T-80333
1-(2,3,4-Trihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethylene, T-60344
ent-2α,3α,16-Trihydroxy-8(14)-pimaren-15-one, *in* P-60154
2,3,12-Trihydroxy-4,7-pregnadien-20-one, T-60345
3β,16β,20*S*-Trihydroxy-5α-pregnane-20-carboxylic acid 22,16-lactone, *see* L-60042
2,3,12-Trihydroxy-4,7,16-pregnatrien-20-one, T-60346
4′,5,7-Trihydroxy-6-prenyisoflavone, *see* W-80002
4′,5,7-Trihydroxy-3′-prenylflavanone, T-80334
2′,4′,7-Trihydroxy-3′-prenylisoflavan, *see* P-80077
1,3,6-Trihydroxy-2-prenylxanthone, *see* T-80325
2,3,9-Trihydroxypterocarpan, T-80335
3,4,9-Trihydroxypterocarpan, T-80336
3,9,10-Trihydroxypterocarpan, T-80338
3,6*a*,9-Trihydroxypterocarpan, T-80337
4′,7,8-Trihydroxypterocarpan, *see* T-80336
5,9,10-Trihydroxy-2*H*-pyrano[2,3,4-*kl*]xanthen-2-one, T-70273
2,4,6-Trihydroxypyridine, *see* D-70341
2,11,12-Trihydroxy-6,7-seco-8,11,13-abietatriene-6,7-dial 11,6-hemiacetal, T-80339
12,20,25-Trihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, T-70274
20,25,26-Trihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, T-70275
3β,23,27-Trihydroxy-28,20-taraxastanolide, *in* H-70221
3,4′,5-Trihydroxy-3′,6,7,8-tetramethoxyflavone, *in* H-80028
3′,5,5′-Trihydroxy-3,4′,7,8-tetramethoxyflavone, *in* H-70021
3′,5,5′-Trihydroxy-4′,6,7,8-tetramethoxyflavone, *in* H-80029
3′,5,7-Trihydroxy-3,4′,5′,8-tetramethoxyflavone, *in* H-70021
3′,5,7-Trihydroxy-4′,5′,6,8-tetramethoxyflavone, *in* H-80029
12,15,20-Trihydroxy-3,7,11,23-tetraoxo-8-lanosten-26-oic acid, T-80340
3,23,25-Trihydroxy-7-tiracallen-24-one, T-60347
23ξ,24ξ,25-Trihydroxy-7-tirucallen-3-one, *in* P-50204
α,2,5-Trihydroxytoluene, *see* D-70287
α,3,4-Trihydroxytoluene, *see* D-80284
5,6,7-Trihydroxy-3-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* H-80071
5,7,8-Trihydroxy-3-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, *see* H-80070
4′,5,7-Trihydroxy-3′,6,8-trimethoxyflavone, T-80341
2′,3′,5-Trihydroxy-3,7,8-trimethoxyflavone, *in* H-70079
2′,5,5′-Trihydroxy-3,7,8-trimethoxyflavone, *in* H-70080
2′,5′,6-Trihydroxy-3,5,7-trimethoxyflavone, *in* H-60064
3′,4′,5-Trihydroxy-3,6,7-trimethoxyflavone, *in* H-80067
3′,4′,5-Trihydroxy-5′,6,7-trimethoxyflavone, *in* H-70081
3′,5,7-Trihydroxy-4′,5′,6-trimethoxyflavone, *in* H-70081
2′,6,8-Trihydroxy-3′,4′,7-trimethoxyisoflavan, *in* H-80068
3′,5,7-Trihydroxy-4′,5′,6-trimethoxyisoflavone, *in* H-80071
3β,7α,15α-Trihydroxy-4,4,14α-trimethyl-11-oxo-5α-chol-8-en-24-oic acid, *see* L-60037
2,3,20-Trihydroxy-1(15),8(19)-trinervitadiene, *see* T-70299
3,9,13-Trihydroxy-11,15(17)-trinervitadiene, *see* T-70297
3β,12β,28-Trihydroxy-7,11,15-trioxo-25,26,27-trisnor-8-lanosten-24-oic acid, *in* L-60036
2,2′,2″-Trihydroxytriphenylamine, *see* N-70039
4,4′,4″-Trihydroxytriphenylamine, *see* N-70040
4′,5,7-Trihydroxy-3′,6,8-triprenylflavanone, *see* A-80151
4′,5,7-Trihydroxy-3′,6,8-triprenylisoflavone, *see* E-70058
2α,3α,24-Trihydroxy-12,20(30)-ursadien-28-oic acid, *in* D-60381
3β,6β,19α-Trihydroxy-12-ursene-23,28-dioic acid, *in* T-80129
2,3,19-Trihydroxy-12-ursen-28-oic acid, T-80342
2,3,23-Trihydroxy-12-ursen-28-oic acid, T-80343
3,11,12-Trihydroxy-20-ursen-28-oic acid, T-80344
3,19,24-Trihydroxy-12-ursen-28-oic acid, T-60348
3,19,24-Trihydroxy-12-ursen-28-oic acid, T-80345
3,6,19-Trihydroxy-12-ursen-28-oic acid, T-80346
1,3,7-Trihydroxy-9*H*-xanthen-9-one, *see* T-80347
1,5,6-Trihydroxy-9*H*-xanthen-9-one, *see* T-60349
1,3,7-Trihydroxyxanthone, T-80347
1,5,6-Trihydroxyxanthone, T-60349
2,3′-2′,3″-Triindolyl, *see* T-60011
▷ 2,4,5-Triiodo-1*H*-imidazole, T-70276
ω,ω′,ω″-Triiodomesitylene, *see* T-80366
3,3′,5-Triiodothyronine, T-60350
Trijugin *A*, T-60351
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Trillarin, *in* S-60045
Trillin, *in* S-60045
2,4,6-Trimercaptopyrimidine, *see* M-80030
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▷ Trimethidinium methosulphate, *in* T-70277
2′,4′,6′-Trimethoxyacetophenone, *in* T-70248
3′,4′,5′-Trimethoxyacetophenone, *in* T-60315
2,3,4-Trimethoxybenzeneacetic acid, *in* T-60340
2,4,5-Trimethoxybenzeneacetic acid, *in* T-60342
3,4,5-Trimethoxybenzeneacetic acid, *in* T-60343
▷ 3,4,5-Trimethoxybenzeneacetonitrile, *in* T-60343
2,3,5-Trimethoxybenzoic acid, *in* T-70250
2,3,5-Trimethoxybenzonitrile, *in* T-70250
2,4,6-Trimethoxybenzophenone, *in* T-80285
5,6,7-Trimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287
5,7,8-Trimethoxy-2*H*-1-benzopyran-2-one, *in* T-80288
3,4,5-Trimethoxybenzyl alcohol, *in* H-80196
2,3,4-Trimethoxybiphenyl, *in* B-70124
3,4,5-Trimethoxybiphenyl, *in* B-80129
2′,4′,6′-Trimethoxychalcone, *in* P-80139
2,4,5-Trimethoxycinnamaldehyde, *see* T-70278
5,6,7-Trimethoxycoumarin, *in* T-80287
5,7,8-Trimethoxycoumarin, *in* T-80288
2′,4′,6′-Trimethoxydihydrochalcone, *in* T-80332
1-(5,7,8-Trimethoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)ethanone, *see* E-80091
3,4,6-Trimethoxy-1,2-dimethylcarbazole, *in* T-70253
5,6,7-Trimethoxyflavone, *in* T-60322
5,7,8-Trimethoxyflavone, *in* T-60321
2′,4′,7-Trimethoxyisoflavone, *in* T-70264
3′,4′,7-Trimethoxyisoflavone, *in* T-80308
4′,6,7-Trimethoxyisoflavone, *in* T-80310
4′,7,8-Trimethoxyisoflavone, *in* T-70265
1,2,8-Trimethoxy-3-methylanthraquinone, *in* T-80322
3,4,6-Trimethoxy-2-methylbenzoic acid, *in* T-80324
2′,6,7-Trimethoxy-4′,5′-methylenedioxyisoflavone, *in* P-80042
3′,4′,8-Trimethoxy-6,7-methylenedioxyisoflavone, *in* P-80046
3′,6,7-Trimethoxy-4′,5′-methylenedioxyisoflavone, *in* P-80044
5,6,7-Trimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-70032
5,6,7-Trimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80043
6,7,8-Trimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80046
5,6,7-Trimethoxy-8-(3-methyl-2-oxobutyl)-2*H*-1-benzopyran-2-one, *see* M-70160
1,4,5-Trimethoxynaphthalene, *in* N-60005
3,6,7-Trimethoxy-1,4-phenanthraquinone, T-80348
2,3,7-Trimethoxyphenanthrene, *in* T-60339
2,4,7-Trimethoxyphenanthrene, *in* P-80080
1,5,6-Trimethoxy-2,7-phenanthrenediol, *in* P-60050
1,5,7-Trimethoxy-2,6-phenanthrenediol, *in* P-60050
5,6,7-Trimethoxy-2,10-phenanthrenediol, *in* P-70035
3,5,7-Trimethoxy-2-phenanthrenol, *in* T-60120
2,3,6-Trimethoxyphenol, *in* B-60014
1,2,4-Trimethoxy-3*H*-phenoxazin-3-one, T-60353
2,3,4-Trimethoxyphenylacetic acid, *in* T-60340
2,4,5-Trimethoxyphenylacetic acid, *in* T-60342
3,4,5-Trimethoxyphenylacetic acid, *in* T-60343
▷ 3,4,5-Trimethoxyphenylacetonitrile, *in* T-60343
1-(2,4,6-Trimethoxyphenyl)-2-buten-1-one, *in* T-80331
1-(2,4,6-Trimethoxyphenyl)-3-phenyl-1-propanone, *in* T-80332
3-(2,4,5-Trimethoxyphenyl)-2-propenal, T-70278
1,2,4-Trimethoxy-5-(2-propenyl)benzene, T-70279
2,3,9-Trimethoxypterocarpan, *in* T-80335
3,4,9-Trimethoxypterocarpan, *in* T-80336
2,4,6-Trimethoxypyridine, *in* D-70341
1,3,7-Trimethoxyxanthone, *in* T-80347

ω-Trimethylacetophenone, *see* D-60443
▷ Trimethylamine oxide, T-60354
N-(γ-Trimethylammoniopropyl)-*N*-methylcamphidinium, *see* T-70277
1,3,6-Trimethyl-5-azauracil, *in* M-60132
3,5,8-Trimethylazuleno[6,5-*b*]furan, *see* L-70031
2,3,5-Trimethylbenzenemethanol, *see* T-80349
3,4,5-Trimethylbenzenemethanol, *see* T-80350
3,4,5-Trimethylbenzoic acid, T-60355
2,5,8-Trimethylbenzotriimidazole, T-60356
2,3,5-Trimethylbenzyl alcohol, T-80349
3,4,5-Trimethylbenzyl alcohol, T-80350
1,7,7-Trimethylbicyclo[2.2.1]heptane-2,5-diol, T-70280
4,7,7-Trimethylbicyclo[4.1.0]heptan-2-one, *see* C-60019
7,11,11-Trimethylbicyclo[8.1.0]undeca-2,6-diene-3-carboxaldehyde, *see* I-60088
1,2,3-Trimethyl-9*H*-carbazole, T-60357
1,2,4-Trimethyl-9*H*-carbazole, T-60358
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▷ Xanthotoxin, X-60001
▷ Xanthotoxol, X-60002
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Yomogin, Y-70001
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Yucalexin B-22, *see* D-80285
Yucalexin B′-11, *see* H-80216
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$CBrF_3S$
Trifluoromethanesulfenyl bromide, T-60280

$CClF_3O_2S$
Trifluoromethanesulfonic acid; Chloride, *in* T-70241

$CClNO_3S$
▷ Sulfuryl chloride isocyanate, S-60062

CFN
▷ Cyanogen fluoride, C-80169

CF_3IS
Trifluoromethanesulfenyl iodide, T-60282

CF_4O_2S
Trifluoromethanesulfonic acid; Fluoride, *in* T-70241

CF_4S
▷ Trifluoromethanesulfenyl fluoride, T-60281

CF_8S
Pentafluoro(trifluoromethyl)sulfur, P-60041

$CHBrN_4$
5-Bromo-1*H*-tetrazole, B-80262

CHClFI
Chlorofluoroiodomethane, C-80056

$CHClN_4$
5-Chlorotetrazole, C-80113

CHClOS
Carbonochloridothioic acid, C-60013

$CHFN_4$
5-Fluoro-1*H*-tetrazole, F-80069

CHF_3OS
Trifluoromethanesulfenic acid, T-60279

CHF_3O_3S
Trifluoromethanesulfonic acid, T-70241

$CHIN_4$
5-Iodo-1*H*-tetrazole, I-80042

CHNO
▷ Cyanic acid, C-80167
▷ Fulminic acid, F-80086
▷ Isocyanic acid, I-80057

CH_2BrClO_2S
Bromomethanesulfonic acid; Chloride, *in* B-60291
Chloromethanesulfonyl bromide, *in* C-70086

CH_2BrIO_2S
Iodomethanesulfonic acid; Bromide, *in* I-60048

$CH_2Br_2O_2S$
Bromomethanesulfonic acid; Bromide, *in* B-60291

CH_2ClI
Chloroiodomethane, C-80068

$CH_2Cl_2O_2S$
▷ Chloromethanesulfonyl chloride, *in* C-70086

$CH_2F_3NO_2S$
Trifluoromethanesulfonic acid; Amide, *in* T-70241
▷ Trifluoromethanesulfonic acid; Me ester, *in* T-70241

$CH_2N_2OS_3$
1,3λ^4,δ^2,5,2,4-Trithiadiazine; 1-Oxide, *in* T-70327

$CH_2N_2O_3S$
Diazomethanesulfonic acid, D-80065

$CH_2N_2S_3$
1,3λ^4,δ^2,5,2,4-Trithiadiazine, T-70327

CH_2N_4O
2-Tetrazolin-5-one, T-60175

CH_2N_4S
Tetrazole-5-thione, T-60174

CH_2OS
Methanethial; *S*-Oxide, *in* M-70037

CH_2OSe
Methaneselenoic acid, M-70035

CH_2S
Methanethial, M-70037

CH_2S_3
Carbonotrithioic acid, C-80019

CH_2Se
▷ Selenoformaldehyde, S-70029

CH_3BrO
Bromomethanol, B-80212

CH_3BrO_3S
Bromomethanesulfonic acid, B-60291

CH_3ClO
Chloromethanol, C-80070

CH_3ClO_3S
Chloromethanesulfonic acid, C-70086

CH_3IO
Iodomethanol, I-80033

CH_3IO_3S
Iodomethanesulfonic acid, I-60048

CH_3N
▷ Methanimine, M-70038

CH_3NO_2
Carbonimidic acid, C-70019

CH_3NSe
Methaneselenoamide, *in* M-70035

$CH_3N_3O_2S$
▷ Methanesulfonyl azide, M-60033

CH_3N_5
▷ 5-Amino-1*H*-tetrazole, A-70202

$CH_4N_2O_3$
O,O'-Carbonylbis(hydroxylamine), C-60015

$CH_4N_2O_3S$
Aminoiminomethanesulfonic acid, A-60210

$CH_4N_2S_2$
Dithiocarbazic acid, D-60509

CH_4N_2Se
▷ Selenourea, S-70031

CH_5NO_3S
Aminomethanesulfonic acid, A-60215

CS
▷ Carbon monosulfide, C-70020

$C_2BrF_3N_2$
▷ 3-Bromo-3-(trifluoromethyl)-3*H*-diazirine, B-70275

C_2BrF_4I
1-Bromo-1,1,2,2-tetrafluoro-2-iodoethane, B-80260

$C_2Br_2ClF_3$
▷ 1,1-Dibromo-1-chloro-2,2,2-trifluoroethane, D-80084
1,2-Dibromo-1-chloro-1,2,2-trifluoroethane, D-80085

$C_2ClF_3N_2$
▷ 3-Chloro-3-(trifluoromethyl)-3*H*-diazirine, C-70169

C_2ClF_3O
Chlorotrifluorooxirane, C-60140

$C_2Cl_2F_2O$
2,2-Dichloro-3,3-difluorooxirane, D-60128

$C_2Cl_2F_3I$
▷ 1,1-Dichloro-1,2,2-trifluoro-2-iodoethane, D-80142
1,2-Dichloro-1,1,2-trifluoro-2-iodoethane, D-80143

$C_2Cl_2F_4$
▷ 1,1-Dichloro-1,2,2,2-tetrafluoroethane, D-80134

$C_2Cl_2O_2S_2$
Bis(chlorocarbonyl) disulfide, B-80142

$C_2Cl_4O_2$
▷ Trichloromethyl chloroformate, T-70223

$C_2F_2I_2$
1,1-Difluoro-2,2-diiodoethylene, D-60183

C_2F_3N
Trifluoroisocyanomethane, T-60278

$C_2F_3NO_3$
▷ Trifluoroacetyl nitrite, T-60274

$C_2F_4I_2$
1,1,2,2-Tetrafluoro-1,2-diiodoethane, T-80050

$C_2F_4N_2$
▷ 3-Fluoro-3-(trifluoromethyl)-3*H*-diazirine, F-70037

C_2F_4O
▷ Tetrafluorooxirane, T-60049

$C_2F_4OS_2$
2,2,4,4-Tetrafluoro-1,3-dithietane; 1-Oxide, *in* T-60048

$C_2F_4O_2S$
Trifluoroethenesulfonic acid; Fluoride, *in* T-60277

$C_2F_4O_2S_2$
2,2,4,4-Tetrafluoro-1,3-dithietane; 1,1-Dioxide, *in* T-60048

$C_2F_4O_3S_2$
2,2,4,4-Tetrafluoro-1,3-dithietane; 1,1,3-Trioxide, *in* T-60048

$C_2F_4O_4S_2$
2,2,4,4-Tetrafluoro-1,3-dithietane; 1,1,3,3-Tetroxide, *in* T-60048

$C_2F_4S_2$
2,2,4,4-Tetrafluoro-1,3-dithietane, T-60048

C_2F_5N
(Trifluoromethyl)carbonimidic difluoride, T-60288

$C_2F_6N_2O_2$
1,1,1-Trifluoro-*N*-(nitrosooxy)-*N*-(trifluoromethyl)methanamine, *in* B-60180

$C_2F_6O_3S$
Trifluoromethyl trifluoromethanesulfonate, *in* T-70241

$C_2F_6O_5S_2$
Trifluoromethanesulfonic acid; Anhydride, *in* T-70241

$C_2F_7NO_4S_2$
Perfluoromethanesulfonimide, P-70042

$C_2F_8S_2$
Difluoro(trifluoromethanethiolato)(trifluoromethyl)-sulfur, *in* T-60281

$C_2HBrClF_3$
▷ 1-Bromo-2-chloro-1,1,2-trifluoroethane, B-80186

$C_2HBrCl_2F_2$
2-Bromo-1,2-dichloro-1,1-difluoroethane, B-80193

C_2HBrF_2
1-Bromo-1,2-difluoroethylene, B-80194

C_2HBrF_4
1-Bromo-1,1,2,2-tetrafluoroethane, B-80259

$C_2HBr_2F_3$
2,2-Dibromo-1,1,1-trifluoroethane, D-80106

C_2HClF_2
1-Chloro-1,2-difluoroethene, C-80048
▷ 2-Chloro-1,1-difluoroethene, C-80049

C_2HClF_3I
1-Chloro-1,1,2-trifluoro-2-iodoethane, C-80119

C_2HCl_2F
1,1-Dichloro-2-fluoroethene, D-80118

$C_2HCl_2F_3$
1,1-Dichloro-1,2,2-trifluoroethane, D-80139
▷ 1,2-Dichloro-1,1,2-trifluoroethane, D-80140
2,2-Dichloro-1,1,1-trifluoroethane, D-80141

$C_2HCl_3F_2$
1,1,2-Trichloro-1,2-difluoroethane, T-80225
1,2,2-Trichloro-1,1-difluoroethane, T-80226

C_2HCl_4F
1,1,1,2-Tetrachloro-2-fluoroethane, T-80015
1,1,2,2-Tetrachloro-1-fluoroethane, T-80016

C_2HF_3
▷ Trifluoroethene, T-80274

C_2HF_3O
Trifluorooxirane, T-60305

$C_2HF_3O_2$
▷ Trifluoroacetic acid, T-80267

$C_2HF_3O_3S$
Trifluoroethenesulfonic acid, T-60277

C_2HF_6NO
N,N-Bis(trifluoromethyl)hydroxylamine, B-60180

C_2HN_5S
3-Azido-1,2,4-thiadiazole, A-60351

$C_2H_2BrF_2I$
1-Bromo-1,1-difluoro-2-iodoethane, B-80196

$C_2H_2BrF_3$
2-Bromo-1,1,1-trifluoroethane, B-80265

$C_2H_2Cl_2$
▷ 1,1-Dichloroethylene, D-80116

$C_2H_2FN_3O_2S$
1,2,4-Triazole-3(5)-sulfonic acid; Fluoride, *in* T-80211

$C_2H_2F_2O$
2,3-Difluorooxirane, D-60187

$C_2H_2F_2O_3S$
4,4-Difluoro-1,2-oxathietane 2,2-dioxide, D-60186

$C_2H_2F_3I$
1,1,1-Trifluoro-2-iodoethane, T-80276

$C_2H_2F_3NO$
Trifluoroacetamide, *in* T-80267

$C_2H_2F_4$
▷ 1,1,2,2-Tetrafluoroethane, T-80051

$C_2H_2N_2O_2$
1,3-Diazetidine-2,4-dione, D-60057

$C_2H_2N_2O_3$
1,2,4-Oxadiazolidine-3,5-dione, O-70060
1,3,4-Oxadiazolidine-2,5-dione, O-70061
1,2,4-Oxazolidine-3,5-dione, O-70070

$C_2H_2N_2O_4$
2*H*-1,5,2,4-Dioxadiazine-3,6(4*H*)dione, D-60466

$C_2H_2N_2S_3$
▷ 5-Mercapto-1,3,4-thiadiazoline-2-thione, M-70031

$C_2H_2N_4$
1,2,4,5-Tetrazine, T-60170

$C_2H_2N_4O_2$
1,2-Dihydro-1,2,4,5-tetrazine-3,6-dione, D-70268

C_2H_2O
Ethynol, E-80070

$C_2H_2O_5$
Dicarbonic acid, D-70111

$C_2H_2S_4$
Ethanebis(dithioic)acid, E-60040

$C_2H_2Se_2$
1,2-Diselenete, D-60498

$C_2H_3AsF_6N_2S_2$
5-Methyl-1,3,2,4-dithiazolium(1+); Hexafluoroarsenate, *in* M-70061

$C_2H_3BrN_4$
5-Bromo-1*H*-tetrazole; 1-Me, *in* B-80262

$C_2H_3ClN_2O$
3-Chloro-3-methoxy-3*H*-diazirine, C-70087

$C_2H_3ClN_2S_2$
5-Methyl-1,3,2,4-dithiazolium(1+); Chloride, *in* M-70061

C_2H_3ClOS
Carbonochloridothioic acid; *O*-Me, *in* C-60013

$C_2H_3Cl_2F$
1,1-Dichloro-1-fluoroethane, D-80117

$C_2H_3FN_2O$
▷ 3-Fluoro-3-methoxy-3*H*-diazirine, F-60050

$C_2H_3F_3$
▷ 1,1,1-Trifluoroethane, T-80273

$C_2H_3F_3OS$
Methyl trifluoromethanesulfenate, *in* T-60279
Trifluoro(methylsulfinyl)methane, *in* M-70145

$C_2H_3F_3O_2S$
Trifluoro(methylsulfonyl)methane, *in* M-70145

$C_2H_3F_3S$
Methyl trifluoromethyl sulfide, M-70145

C_2H_3N
2*H*-Azirine, A-70292
Ethenimine, E-80058
Ethynamine, E-60056

C_2H_3NO
Fulminic acid; Trimolecular Me ester, *in* F-80086

$C_2H_3NO_2$
Methoxy isocyanate, M-80045

$C_2H_3NS_2$
Methanesulfenyl thiocyanate, M-60032

C_2H_3NSe
Methyl selenocyanate, M-60127

$C_2H_3N_2S_2^{\oplus}$
5-Methyl-1,3,2,4-dithiazolium(1+), M-70061

$C_2H_3N_3O_3S$
1,2,4-Triazole-3(5)-sulfonic acid, T-80211

$C_2H_3N_3S$
▷ 1,2-Dihydro-3*H*-1,2,4-triazole-3-thione, D-60298

$C_2H_4BrNO_2$
1-Bromo-2-nitroethane, B-60303

C_2H_4ClI
1-Chloro-1-iodoethane, C-60106
1-Chloro-2-iodoethane, C-70078

$C_2H_4IN_3$
1-Azido-2-iodoethane, A-60346

$C_2H_4N_2O$
1,2-Diazetidin-3-one, D-70055

$C_2H_4N_2O_4$
▷ Oxalohydroxamic acid, O-60048

$C_2H_4N_2S_2$
▷ Ethanedithioamide, E-60041

$C_2H_4N_4O_2$
▷ Tetrahydro-1,2,4,5-tetrazine-3,6-dione, T-70097

$C_2H_4N_4O_2S$
1,2,4-Triazole-3(5)-sulfonic acid; Amide, *in* T-80211

$C_2H_4N_4S$
2,5-Diamino-1,3,4-thiadiazole, D-60049
1*H*-Tetrazole-5-thiol; *S*-Me, *in* T-60174
Tetrazole-5-thione; 1-Me, *in* T-60174

$C_2H_4N_6$
3,6-Diamino-1,2,4,5-tetrazine, D-70045

C_2H_4OS
Mercaptoacetaldehyde, M-80017

$C_2H_4O_2$
▷ 1,2-Dioxetane, D-60469

$C_2H_4O_4S$
Formylmethanesulfonic acid, F-80076

$C_2H_4O_5S$
Sulfoacetic acid, S-80050

C_2H_5NO
▷ Acetamide, A-70019

$C_2H_5NO_3$
C-Methoxycarbohydroxamic acid, M-70044

$C_2H_5N_3O$
▷ 2-Azidoethanol, A-70287

$C_2H_5N_3O_2$
Biuret, B-60190
▷ Semioxamazide, S-60020

$C_2H_5N_5$
5-Amino-1-methyl-1*H*-tetrazole, *in* A-70202
5-Amino-2-methyl-2*H*-tetrazole, *in* A-70202
5-Methylamino-1*H*-tetrazole, *in* A-70202

$C_2H_6N_2O$
▷ Acetamidoxime, A-60016

$C_2H_6N_2O_2$
▷ *N*-Nitrodimethylamine, N-80045

$C_2H_6N_2O_3S$
Aminoiminomethanesulfonic acid; *N*-Me, *in* A-60210

$C_2H_6N_2S_2$
Dithiocarbazic acid; Me ester, *in* D-60509

$C_2H_6N_2Se$
Selenourea; *N*-Me, *in* S-70031

C_2H_6OS
(Methylthio)methanol, M-70138

$C_2H_6O_2S_2$
2-Mercaptoethanesulfinic acid, M-60022

$C_2H_6O_6S_2$
Bis(methylsulfonyl) peroxide, B-70154

C_2H_7NO
O,N-Dimethylhydroxylamine, D-70418

$C_2H_7NO_2$
O-(2-Hydroxyethyl)hydroxylamine, H-60134

$C_2H_7NO_3S$
(Methylamino)methanesulfonic acid, *in* A-60215

$C_2H_8N_2$
▷ 1,1-Dimethylhydrazine, D-70416

$C_2H_9N_3$
2-Hydrazinoethylamine, H-70096

$C_2H_{10}N_4$
1,2-Dihydrazinoethane, D-60192

C_2N_2
Diisocyanogen, D-70362

$C_2N_2Se_3$
Dicyanotriselenide, D-60165

C_2O_2
Dicarbon dioxide, D-80114

C_3AlCl_7
Trichlorocyclopropenylium; Tetrachloroaluminate, *in* T-70221

C_3BrF_2I
1-Bromo-3,3-difluoro-2-iodocyclopropene, B-80195

C_3BrF_3
1-Bromo-2,3,3-trifluorocyclopropene, B-80264

C_3BrF_7
▷ 1-Bromo-1,1,2,2,3,3,3-heptafluoropropane, B-80206
2-Bromo-1,1,1,2,3,3,3-heptafluoropropane, B-80207

$C_3Br_2F_6$
1,3-Dibromo-1,1,2,2,3,3-hexafluoropropane, D-80094

$C_3Br_3N_3O_2$
3,4,5-Tribromo-1*H*-pyrazole; 1-Nitro, *in* T-60246

$C_3ClF_2N_3$
2-Chloro-4,6-difluoro-1,3,5-triazine, C-60052
6-Chloro-3,5-difluoro-1,2,4-triazine, C-60053

C_3ClF_3
1-Chloro-2,3,3-trifluorocyclopropene, C-80118

C_3ClF_5
1-Chloro-1,2,3,3,3-pentafluoro-1-propene, C-80090

$C_3Cl_2F_4$
1,1-Dichloro-2,3,3,3-tetrafluoro-1-propene, D-80135
1,2-Dichloro-1,3,3,3-tetrafluoro-1-propene, D-80136

$C_3Cl_2F_6$
1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane, D-80120
1,3-Dichloro-1,1,2,2,3,3-hexafluoropropane, D-80121
2,2-Dichloro-1,1,1,3,3,3-hexafluoropropane, D-80122

$C_3Cl_3^{\oplus}$
Trichlorocyclopropenylium, T-70221

$C_3Cl_3F_5$
1,1,1-Trichloro-2,2,3,3,3-pentafluoropropane, T-80228
1,1,3-Trichloro-1,2,2,3,3-pentafluoropropane, T-80229
1,2,2-Trichloro-1,1,3,3,3-pentafluoropropane, T-80230
1,2,3-Trichloro-1,1,2,3,3-pentafluoropropane, T-80231

$C_3Cl_3N_3$
Trichloro-1,2,3-triazine, T-80232

$C_3Cl_4F_4$
1,1,1,2-Tetrachloro-2,3,3,3-tetrafluoropropane, T-80018
1,1,1,3-Tetrachloro-2,2,3,3-tetrafluoropropane, T-80019
1,1,2,2-Tetrachloro-1,3,3,3-tetrafluoropropane, T-80020
1,1,2,3-Tetrachloro-1,2,3,3-tetrafluoropropane, T-80021
1,1,3,3-Tetrachloro-1,2,2,3-tetrafluoropropane, T-80022

$C_3Cl_6O_3$
Bis(trichloromethyl) carbonate, B-70163

C_3Cl_8
Octachloropropane, O-80004

C_3Cl_9Sb
Trichlorocyclopropenylium; Hexachloroantimonate, *in* T-70221

$C_3F_2I_2$
3,3-Difluoro-1,2-diiodocyclopropene, D-80160

$C_3F_3N_3$
Trifluoro-1,2,3-triazine, T-70245

C_3F_5N
2,2-Difluoro-3-(trifluoromethyl)-2*H*-azirine, D-80165
2,3-Difluoro-2-(trifluoromethyl)-2*H*-azirine, D-80166

$C_3F_6N_2$
3,3-Bis(trifluoromethyl)-3*H*-diazirine, B-60178

$C_3F_6O_2S$
Bis(trifluoromethyl)sulfene, B-80162

$C_3F_6O_4S$
Trifluoroacetyl trifluoromethanesulfonate, *in* T-70241

C_3F_7I
1,1,2,2,3,3,3-Heptafluoro-1-iodopropane, H-80026

C_3F_7NO
3,3,4,4-Tetrafluoro-2-(trifluoromethyl)-1,2-oxazetidine, T-60051

C_3F_9N
Tris(trifluoromethyl)amine, T-60406

$C_3HBrINS$
2-Bromo-4-iodothiazole, B-60287
2-Bromo-5-iodothiazole, B-60288
4-Bromo-2-iodothiazole, B-60289
5-Bromo-2-iodothiazole, B-60290

C_3HBr_2NS
2,4-Dibromothiazole, D-60109
2,5-Dibromothiazole, D-60110
4,5-Dibromothiazole, D-60111

$C_3HBr_2N_3$
4,5-Dibromo-1,2,3-triazine, D-70100
4,5-Dibromo-1,2,3-triazine, D-80105

$C_3HBr_3N_2$
▷ 2,4,5-Tribromo-1*H*-imidazole, T-60245
3,4,5-Tribromo-1*H*-pyrazole, T-60246

C_3HClF_4
1-Chloro-2,3,3,3-tetrafluoro-1-propene, C-80109

C_3HCl_2NS
2,4-Dichlorothiazole, D-60154
2,5-Dichlorothiazole, D-60155
4,5-Dichlorothiazole, D-60156

C_3HCl_5
Pentachlorocyclopropane, P-70018

C_3HF_3
1,3,3-Trifluorocyclopropene, T-80271

C_3HF_5
1,1,3,3,3-Pentafluoro-1-propene, P-80028

C_3HI_2NS
2,4-Diiodothiazole, D-60388
2,5-Diiodothiazole, D-60389

$C_3HI_3N_2$
▷ 2,4,5-Triiodo-1*H*-imidazole, T-70276

$C_3HN_3O_5$
3,5-Dinitroisoxazole, D-70452

$C_3H_2BrN_3$
5-Bromo-1,2,3-triazine, B-70273
5-Bromo-1,2,3-triazine, B-80263

$C_3H_2BrN_3O_2$
3(5)-Bromo-5(3)-nitro-1*H*-pyrazole, B-60305
4-Bromo-3(5)-nitro-1*H*-pyrazole, B-60304

$C_3H_2Br_2$
1,2-Dibromocyclopropene, D-60094

$C_3H_2Br_2N_2$
2,4(5)-Dibromo-1*H*-imidazole, D-70093
4,5-Dibromo-1*H*-imidazole, D-60100

$C_3H_2ClF_3$
2-Chloro-3,3,3-trifluoro-1-propene, C-60141

$C_3H_2ClF_3O$
3,3,3-Trifluoropropanoic acid; Chloride, *in* T-80284

$C_3H_2ClF_3O_2$
2-Chloro-3,3,3-trifluoropropanoic acid, C-70170

$C_3H_2ClF_5$
1-Chloro-1,1,3,3,3-pentafluoropropane, C-80088
1-Chloro-2,2,3,3,3-pentafluoropropane, C-80089

$C_3H_2ClN_3O_2$
6-Chloro-1,2,4-triazine-3,5(1*H*,3*H*)-dione, C-80114
6-Chloro-1,3,5-triazine-2,4(1*H*,3*H*)-dione, C-80115

$C_3H_2Cl_2N_2$
4,5-Dichloro-1*H*-imidazole, D-70122

$C_3H_2Cl_2O$
2,3-Dichloro-2-propenal, D-80127
▷ 3,3-Dichloro-2-propenal, D-80128

$C_3H_2Cl_4O_2$
Chloromethanol; Trichloroacetyl, *in* C-80070

$C_3H_2F_4O$
2-Fluoro-3-(trifluoromethyl)oxirane, F-80070

$C_3H_2F_6$
1,1,1,2,2,3-Hexafluoropropane, H-80049
1,1,1,3,3,3-Hexafluoropropane, H-80050

C_3H_2INS
2-Iodothiazole, I-60064
4-Iodothiazole, I-60065
5-Iodothiazole, I-60066

$C_3H_2N_2O_2S$
2-Thioxo-4,5-imidazolidinedione, T-70187

$C_3H_2N_3$
▷ 2-Diazo-2*H*-imidazole, D-70060

$C_3H_2N_4$
4-Cyano-1,2,3-triazole, *in* T-60239
▷ 4-Diazo-4*H*-imidazole, D-70061

$C_3H_2N_6$
Tetrazolo[1,5-*b*][1,2,4]triazine, T-80164

$C_3H_2O_3$
2,3-Dihydroxy-2-cyclopropen-1-one, D-70290

C_3H_2S
1,2-Propadiene-1-thione, P-70117

$C_3H_2S_3$
2,3-Dimercapto-2-propene-1-thione, D-80410

$C_3H_2S_5$
4,5-Dimercapto-1,3-dithiole-2-thione, D-80409

$C_3H_3BrN_2$
▷ 2-Bromo-1*H*-imidazole, B-70220
4(5)-Bromo-1*H*-imidazole, B-70221
3(5)-Bromopyrazole, B-80253
▷ 4-Bromopyrazole, B-80254

$C_3H_3Br_2Cl$
1,1-Dibromo-2-chlorocyclopropane, D-80082

$C_3H_3Br_3$
1,2,3-Tribromocyclopropane, T-70211

$C_3H_3ClN_2$
2-Chloro-1*H*-imidazole, C-70076
4(5)-Chloro-1*H*-imidazole, C-70077
3-Chloro-1*H*-pyrazole, C-70155
▷ 4-Chloro-1*H*-pyrazole, C-70156

$C_3H_3ClN_2O$
4-Chloro-5-methylfurazan, C-60114

$C_3H_3ClN_2O_2$
2-Chloro-2,3-dihydro-1*H*-imidazole-4,5-dione, C-60054
4-Chloro-3-methylfuroxan, *in* C-60114

C_3H_3ClO
▷ 2-Propenoic acid; Chloride, *in* P-70121

$C_3H_3Cl_2F_3$
2,2-Dichloro-1,1,1-trifluoropropane, D-80144
2,3-Dichloro-1,1,1-trifluoropropane, D-80145
3,3-Dichloro-1,1,1-trifluoropropane, D-80146

$C_3H_3Cl_2F_3O$
2,2-Dichloro-3,3,3-trifluoro-1-propanol, D-60161

$C_3H_3Cl_2N_2O_2$
3-Chloro-4-methylfuroxan, *in* C-60114

$C_3H_3Cl_3$
1,2,3-Trichlorocyclopropane, T-70220
1,1,2-Trichloro-1-propene, T-60254

$C_3H_3F_3O$
(Trifluoromethyl)oxirane, T-60294
3,3,3-Trifluoropropanal, T-80282

$C_3H_3F_3O_2$
Trifluoroacetic acid; Me ester, *in* T-80267
3,3,3-Trifluoropropanoic acid, T-80284

$C_3H_3F_6NO$
1,1,1,1′,1′,1′-Hexafluoro-*N*-methoxydimethylamine, *in* B-60180

$C_3H_3IN_2$
4(5)-Iodo-1*H*-imidazole, I-70042
3(5)-Iodopyrazole, I-80040
4-Iodopyrazole, I-80041

C_3H_3N
▷ Vinyl cyanide, *in* P-70121

$C_3H_3NO_3S_2$
4-Thiazolesulfonic acid, T-60198
5-Thiazolesulfonic acid, T-60199

$C_3H_3NO_4$
2*H*-1,5,2-Dioxazine-3,6(4*H*)-dione, D-70464

$C_3H_3NS_2$
2(3*H*)-Thiazolethione, T-60200

$C_3H_3N_3O$
2-Nitrosoimidazole, N-80059

$C_3H_3N_3O_2$
3-Azido-2-propenoic acid, A-70290
1*H*-1,2,3-Triazole-4-carboxylic acid, T-60239

$C_3H_3N_3O_3$
▷ Cyanuric acid, C-60179

$C_3H_3N_5$
3(5)-Azidopyrazole, A-70291

$C_3H_3N_7O_2$
7,8-Dihydrotetrazolo[1,5-*b*][1,2,4]triazine; 8-Nitro, *in* D-80256

$C_3H_4BrClO_2$
Bromomethanol; Chloroacetyl, *in* B-80212

C_3H_4ClNO
▷ 1-Chloro-2-isocyanatoethane, C-80069

C_3H_4ClNS
▷ 1-Chloro-2-isothiocyanoethane, C-70081

$C_3H_4Cl_2O_2$
Chloromethanol; Chloroacetyl, *in* C-80070

$C_3H_4F_3NO$
3,3,3-Trifluoropropanoic acid; Amide, *in* T-80284

$C_3H_4I_2N_6$
1,3-Diiodo-2,2-diazidopropane, D-60387

$C_3H_4N_2$
Diazocyclopropane, D-60060
▷ 1*H*-Pyrazole, P-70152

$C_3H_4N_2O$
4-Aminoisoxazole, A-80096
2-Diazopropanal, D-80066

$C_3H_4N_2OS$
▷ 2-Thioxo-4-imidazolidinone, T-70188

$C_3H_4N_2O_2$
2-Propyn-1-amine; *N*-Nitro, *in* P-60184
3,5-Pyrazolidinedione, P-80200

$C_3H_4N_2O_3$
2,3-Dihydro-2-hydroxy-1*H*-imidazole-4,5-dione, D-60243
5-Hydroxy-2,4-imidazolidinedione, H-60156
1,2,4-Oxadiazolidine-3,5-dione; 4-Me, *in* O-70060

$C_3H_4N_2O_4$
1,2-Dinitrocyclopropane, D-80494

$C_3H_4N_2O_5$
1,1-Dinitro-2-propanone, D-70454

$C_3H_4N_2S$
2-Cyanoethanethioamide, C-70209
1,3-Dihydro-2*H*-imidazole-2-thione, D-80215

$C_3H_4N_2S_3$
3-Methyl-1,3,4-thiadiazolidine-2,5-dithione, *in* M-70031
5-Methylthio-1,3,4-thiadiazole-2(3*H*)-thione, *in* M-70031

$C_3H_4N_4$
▷ 3-Amino-1,2,4-triazine, A-70203

$C_3H_4N_4O$
4-Amino-1,3,5-triazin-2(1*H*)-one, A-80149
1*H*-1,2,3-Triazole-4-carboxylic acid; Amide, *in* T-60239

$C_3H_4N_4S$
4-Amino-1,3,5-triazine-2(1*H*)-thione, A-80148

$C_3H_4N_6$
7,8-Dihydrotetrazolo[1,5-*b*][1,2,4]triazine, D-80256

C_3H_4O
▷ Propenal, P-70119

$C_3H_4O_2$
1,3-Dioxole, D-60473
▷ 2-Propenoic acid, P-70121

$C_3H_4O_3$
3-Oxopropanoic acid, O-60090

$C_3H_4S_2Se$
1,3-Dithiolane-2-selone, D-70525

$C_3H_5BrO_2$
Bromomethanol; Ac, *in* B-80212

$C_3H_5ClN_2$
2-Chloro-4,5-dihydro-1*H*-imidazole, C-80050

C_3H_5ClOS
▷ Carbonochloridothioic acid; *O*-Et, *in* C-60013
Carbonochloridothioic acid; *S*-Et, *in* C-60013

$C_3H_5ClO_2$
Chloromethanol; Ac, *in* C-80070

$C_3H_5ClO_3$
▷ 3-Chloro-2-hydroxypropanoic acid, C-70072

C_3H_5FO
▷ (Fluoromethyl)oxirane, F-70032

$C_3H_5F_2NO_2$
2-Amino-3,3-difluoropropanoic acid, A-60135

$C_3H_5F_3O$
1,1,1-Trifluoro-2-methoxyethane, T-80277

$C_3H_5F_3OS$
Ethyl trifluoromethanesulfenate, *in* T-60279

$C_3H_5F_3O_3S$
Trifluoromethanesulfonic acid; Et ester, *in* T-70241

$C_3H_5F_3O_4S_2$
(Methylsulfonyl)[(trifluoromethyl)sulfonyl]methane, M-70133

$C_3H_5IO_2$
▷ Iodomethanol; Ac, *in* I-80033

$C_3H_5I_2N_3$
2-Azido-1,3-diiodopropane, A-80198

C_3H_5N
2,3-Dihydroazete, D-70172
▷ 2-Propyn-1-amine, P-60184

C_3H_5NO
▷ Acrylamide, *in* P-70121
3-Azetidinone, A-80192
Propenal; Oxime, *in* P-70119

$C_3H_5NO_2$
3-Amino-2-oxetanone, A-80129

$C_3H_5NO_3$
Isonitrosopropanoic acid, *in* O-60090
▷ 3-Nitropropanal, N-60037

C_3H_5NS
2-Propenethioamide, P-70120

$C_3H_5NS_2$
2-Thiazoledinethione, T-60197

$C_3H_5N_3O_2$
Dihydro-1,3,5-triazine-2,4(1*H*,3*H*)-dione, D-60297
▷ 2-Imidazolidinone; 1-Nitroso, *in* I-70005
Tetrahydro-1,2,4-triazine-3,6-dione, T-60099

C_3H_6BrF
1-Bromo-3-fluoropropane, B-70212

$C_3H_6BrNO_2$
1-Bromo-1-nitropropane, B-70258
2-Bromo-2-nitropropane, B-70259

$C_3H_6Br_2$
▷ 1,2-Dibromopropane, D-60105

C_3H_6ClN
2-Chloro-2-propen-1-amine, C-70151

$C_3H_6ClNO_2$
▷ 2-Chloro-2-nitropropane, C-60120

$C_3H_6ClN_4^{\oplus}$
N,N-Dimethylazidochloromethyleniminium(1+), D-70369

$C_3H_6Cl_2N_4$
N,N-Dimethylazidochloromethyleniminium(1+); Chloride, *in* D-70369

C_3H_6FI
1-Fluoro-3-iodopropane, F-70026

$C_3H_6FNO_2$
3-Amino-2-fluoropropanoic acid, A-60162

$C_3H_6F_3N$
3,3,3-Trifluoro-1-propanamine, T-80283

$C_3H_6F_3NO_2S$
Trifluoromethanesulfonic acid; Diethylamide, *in* T-70241

$C_3H_6IN_3$
1-Azido-3-iodopropane, A-60347

$C_3H_6IN_3O$
2-Azido-3-iodo-1-propanol, A-80200

$C_3H_6N_2$
4,5-Dihydro-1*H*-imidazole, D-60245
4,5-Dihydro-1*H*-pyrazole, D-70253

$C_3H_6N_2O$
▷ Azetidine; *N*-Nitroso, *in* A-70283
▷ 2-Imidazolidinone, I-70005
4-Imidazolidinone, I-80006

$C_3H_6N_2O_2$
Acetamidoxime; *O*-Formyl, *in* A-60016
3,3-Dimethoxy-3*H*-diazirine, D-80412

$C_3H_6N_4$
1*H*-1,2,3-Triazole-4-methanamine, T-80210

$C_3H_6N_4O$
2-Tetrazolin-5-one; 1-Et, *in* T-60175

$C_3H_6N_4O_2$
2-Amino-3-azidopropanoic acid, A-80058
2-Azido-2-nitropropane, A-60349

$C_3H_6N_4S$
1*H*-Tetrazole-5-thiol; *S*-Et, *in* T-60174
Tetrazole-5-thione; 1,4-Di-Me, *in* T-60174
Tetrazole-5-thione; 1-Et, *in* T-60174

$C_3H_6N_6$
▷ 2,2-Diazidopropane, D-60058

$C_3H_6N_6O_3$
▷ Hexahydro-1,3,5-triazine; 1,3,5-Trinitroso, *in* H-60060

C_3H_6O
▷ Methyloxirane, M-70100

C_3H_6OS
1-Mercapto-2-propanone, M-60028
(Methylthio)acetaldehyde, *in* M-80017
(Methylthio)oxirane, M-80173
Propenylsulfenic acid, P-70123

C_3H_6OSe
3-Selenetanol, S-80022

$C_3H_6O_2$
Dimethyldioxirane, D-70399
1,2-Dioxolane, D-70467

$C_3H_6O_2S$
1,3,2-Dioxathiane, D-80502
▷ 2-Mercaptopropanoic acid, M-60027

$C_3H_6O_3S$
Trimethylene sulfite, *in* D-80502

$C_3H_6O_4S$
Trimethylene sulfate, *in* D-80502

$C_3H_6S_3$
Carbonotrithioic acid; Di-Me ester, *in* C-80019

C_3H_7N
Azetidine, A-70283

C_3H_7NO
▷ Acetamide; *N*-Me, *in* A-70019
2-(Hydroxymethyl)aziridine, H-80194

C_3H_7NOS
2-Mercaptopropanoic acid; Amide, *in* M-60027

$C_3H_7NO_3$
3-Amino-2-hydroxypropanoic acid, A-70160
▷ 3-Nitro-1-propanol, N-60039

$C_3H_7NO_4$
▷ 2-Nitro-1,3-propanediol, N-60038

C_3H_7NSe
N,N-Dimethylmethaneselenoamide, *in* M-70035

$C_3H_7N_3$
2-Azidopropane, A-70289

$C_3H_7N_3O$
1-Azido-1-propanol, A-80204

$C_3H_7N_3O_2$
Allophanic methylamide, *in* B-60190

$C_3H_7N_5$
5-Amino-1-ethyl-1*H*-tetrazole, *in* A-70202
5-Amino-2-ethyl-2*H*-tetrazole, *in* A-70202
1,4-Dihydro-5-imino-3,4-dimethyltetrazole, *in* A-70202
5-Dimethylamino-1*H*-tetrazole, *in* A-70202
5-Ethylamino-1*H*-tetrazole, *in* A-70202
5-Imino-1,3-dimethyl-1*H*,3*H*-tetrazole, *in* A-70202
1-Methyl-5-methylamino-1*H*-tetrazole, *in* A-70202
2-Methyl-5-methylamino-2*H*-tetrazole, *in* A-70202

$C_3H_8N_2O_2$
N,N-Dimethylcarbamohydroxamic acid, D-60414

$C_3H_8N_2O_3S$
Aminoiminomethanesulfonic acid; *N,N*-Di-Me, *in* A-60210

$C_3H_8N_2Se$
Selenourea; N^1,N^1-Di-Me, *in* S-70031
Selenourea; N^1,N^3-Di-Me, *in* S-70031
Selenourea; *N*-Et, *in* S-70031

$C_3H_8O_2$
▷ 1,2-Propanediol, P-70118

$C_3H_8S_2$
2,2-Propanedithiol, P-60175

C_3H_9NO
▷ Trimethylamine oxide, T-60354

$C_3H_9NO_3S$
(Dimethylamino)methanesulfonic acid, *in* A-60215

$C_3H_9N_3$
Hexahydro-1,3,5-triazine, H-60060

C_3OS
3-Thioxo-1,2-propadien-1-one, T-60216

C_4Br_4O
Tetrabromofuran, T-60023

$C_4ClF_3N_2$
3-Chloro-4,5,6-trifluoropyridazine, C-60142
4-Chloro-3,5,6-trifluoropyridazine, C-60143
5-Chloro-2,4,6-trifluoropyrimidine, C-60144

C_4ClF_5
1-Chloro-2,3,3,4,4-pentafluorocyclobutene, C-80087

$C_4Cl_2F_4$
1,2-Dichloro-3,3,4,4-tetrafluorocyclobutene, D-80132
3,4-Dichloro-1,2,3,4-tetrafluorocyclobutene, D-80133

$C_4Cl_2F_4O_2$
Tetrafluorobutanedioic acid; Dichloride, *in* T-80049

$C_4Cl_2O_2$
Chlorofumaric acid; Dichloride, *in* C-80043

$C_4Cl_3F_3$
1,2,3-Trichloro-3,4,4-triflurorocyclobutene, T-80233

$C_4F_2O_3$
3,4-Difluoro-2,5-furandione, *in* D-80159

$C_4F_4O_3$
3,3,4,4-Tetrafluorodihydro-2,5-furandione, *in* T-80049

C_4F_6
▷ (Difluoromethylene)tetrafluorocyclopropane, D-60185

$C_4F_6NS_2$
4,5-Bis(trifluoromethyl)-1,3,2-dithiazol-2-yl, B-70164

$C_4F_6O_2$
1,1,1,4,4,4-Hexafluoro-2,3-butanedione, H-60043

$C_4F_6O_3$
▷ Trifluoroacetic acid; Anhydride, *in* T-80267

$C_4F_6O_4S$
4-[2,2,2-Trifluoro-1-(trifluoromethyl)ethylidene]-1,3,2-dioxathietane 2,2-dioxide, T-60311

C_4F_6S
Bis(trifluoromethyl)thioketene, B-60187

$C_4F_6S_2$
3,4-Bis(trifluoromethyl)-1,2-dithiete, B-60179
Bis[(trifluoromethyl)thio]acetylene, B-80163

C_4F_8O
2,2-Difluoro-3,3-bis(trifluoromethyl)oxirane, D-80158

$C_4F_8O_3S$
4,4-Difluoro-3,3-bis(trifluoromethyl)-1,2-oxathietane 2,2-dioxide, D-60181

C_4F_9NO
Nonafluoromorpholine, N-60056

$C_4HBrF_2O_2$
4-Bromo-4,4-difluoro-2-butynoic acid, B-70202

C_4HBr_3S
2,3,5-Tribromothiophene, T-60247

C_4HClN_2
1-Chloro-1,2-dicyanoethylene, *in* C-80043

C_4HClO_3
3-Chloro-2,5-furandione, *in* C-80043
3-Chloro-4-hydroxy-3-cyclobutene-1,2-dione, C-70071

$C_4HCl_2F_3$
1,4-Dichloro-3,3,4-trifluorocyclobutene, D-80138

C_4HFO_3
3-Fluoro-2,5-furandione, *in* F-80030

$C_4HF_3N_2$
Trifluoropyrazine, T-60306
2,4,6-Trifluoropyrimidine, T-60307
4,5,6-Trifluoropyrimidine, T-60308

$C_4HF_3O_3$
3,3,4-Trifluoro-dihydro-2,5(2*H*,5*H*)-furandione, *in* T-80269

C_4HF_5
3,3,4,4,4-Pentafluoro-1-butyne, P-60032
1,3,3,4,4-Pentafluorocyclobutene, P-60033

C_4HF_8NO
2,2,3,3,5,5,6,6-Octafluoromorpholine, O-60009

C_4HNO
4-Oxo-2-butynenitrile, *in* O-80070

$C_4HN_5O_8$
2,3,4,5-Tetranitro-1*H*-pyrrole, T-60160

$C_4H_2BrNO_2S$
2-Bromo-4-nitrothiophene, B-80239

$C_4H_2Br_2N_2O$
4,5-Dibromo-1*H*-imidazole-2-carboxaldehyde, D-60101

$C_4H_2Br_2N_2O_2$
4,5-Dibromo-1*H*-imidazole-2-carboxylic acid, D-60102

$C_4H_2ClNO_2$
5-Isoxazolecarboxylic acid; Chloride, *in* I-60142

$C_4H_2Cl_2N_2O$
4,5-Dichloro-1*H*-imidazole-2-carboxaldehyde, D-60134
2,6-Dichloro-4(3*H*)-pyrimidinone, D-80130
4,6-Dichloro-2(1*H*)-pyrimidinone, D-80131

$C_4H_2Cl_2N_2O_2$
4,5-Dichloro-1*H*-imidazole-2-carboxylic acid, D-60135

$C_4H_2Cl_3NO$
5-(Trichloromethyl)isoxazole, T-60253

$C_4H_2F_2N_2$
2,3-Difluoropyrazine, D-60188
2,6-Difluoropyrazine, D-60189

$C_4H_2F_2O_4$
1,2-Difluoro-2-butenedioic acid, D-80159

$C_4H_2F_3N$
▷ 2-Trifluoromethylacrylonitrile, *in* T-60295

$C_4H_2F_4$
3,3,4,4-Tetrafluorocyclobutene, T-60043

$C_4H_2F_4O_4$
▷ Tetrafluorobutanedioic acid, T-80049

$C_4H_2F_6S_2$
1,2-Bis[(trifluoromethyl)thio]ethene, B-80164

$C_4H_2N_2O$
5-Cyanoisoxazole, *in* I-60142

$C_4H_2N_2O_2$
Dicyanoacetic acid, D-70149

$C_4H_2N_2O_2S$
1,2,5-Thiadiazole-3,4-dicarboxaldehyde, T-70162

$C_4H_2N_2O_3$
3-Diazo-2,4(5*H*)-furandione, D-70059

$C_4H_2N_2S_2$
(Dimercaptomethylene)malononitrile, *in* D-60395

$C_4H_2N_4OS$
[1,2,5]Thiadiazolo[3,4-*d*]pyridazin-4(5*H*)-one, T-70164

$C_4H_2N_4O_4$
1,2,4,5-Tetrazine-3,6-dicarboxylic acid, T-80163
[1,2,4]Triazolo[1,2-*a*][1,2,4]triazole-1,3,5,7(2*H*,6*H*)-tetrone, T-70209

$C_4H_2N_4O_6$
2,3,4-Trinitro-1*H*-pyrrole, T-60373
2,3,5-Trinitro-1*H*-pyrrole, T-60374

$C_4H_2N_4S$
[1,2,5]Thiadiazolo[3,4-*d*]pyridazine, T-70163

$C_4H_2N_8O_{10}$
Tetrahydro-1,3,4,6-tetranitroimidazo[4,5-*d*]imidazole-2,5-(1*H*,3*H*)-dione, T-70096

$C_4H_2O_2$
2-Butynedial, B-60351

$C_4H_2O_3$
▷ 2-Oxo-3-butynoic acid, O-80069
4-Oxo-2-butynoic acid, O-80070

$C_4H_2S_4$
3,4-Dimercapto-3-cyclobutene-1,2-dithione, D-70364

$C_4H_3BrN_2OS$
5-Bromo-3,4-dihydro-4-thioxo-2(1*H*)-pyrimidinone, B-70205

$C_4H_3BrN_2O_2$
▷ 5-Bromo-2,4-(1*H*,3*H*)-pyrimidinedione, B-60318
6-Bromo-2,4-(1*H*,3*H*)-pyrimidinedione, B-60319

$C_4H_3BrO_2$
5-Bromo-2(5*H*)-furanone, B-80204

$C_4H_3Br_2N_3$
4,5-Dibromo-6-methyl-1,2,3-triazine, D-80096

$C_4H_3ClN_2$
2-Chloropyrazine, C-80108
5-Chloropyrimidine, C-70157

$C_4H_3ClN_2O$
2-Chloropyrazine; 1-Oxide, *in* C-80108
2-Chloropyrazine; 4-Oxide, *in* C-80108
5-Chloropyrimidine; *N*-Oxide, *in* C-70157

$C_4H_3ClN_2OS$
5-Chloro-4-thioxo-2(1*H*)-pyrimidinone, C-70162

$C_4H_3ClN_2O_2$
▷ 5-Chloro-2,4-(1*H*,3*H*)-pyrimidinedione, C-60130
6-Chloro-2,4-(1*H*,3*H*)-pyrimidinedione, C-70158

$C_4H_3ClO_2S_2$
2-Thiophenesulfonic acid; Chloride, *in* T-60213
3-Thiophenesulfonic acid; Chloride, *in* T-60214

$C_4H_3ClO_4$
2-Chloro-2-butenedioic acid, C-80043

C_4H_3ClS
3-Chlorothiophene, C-60136

$C_4H_3FN_2$
5-Fluoropyrimidine, F-80061

$C_4H_3FN_2OS$
5-Fluoro-3,4-dihydro-4-thioxo-2(1*H*)-pyrimidinone, F-70019

$C_4H_3FO_4$
2-Fluoro-2-butenedioic acid, F-80030

$C_4H_3F_3$
1,1,2-Trifluoro-1,3-butadiene, T-80268
1,1,1-Trifluoro-2-butyne, T-60275
1,4,4-Trifluorocyclobutene, T-60276

$C_4H_3F_3N_2$
2-Trifluoromethyl-1*H*-imidazole, T-60289
4(5)-Trifluoromethyl-1*H*-imidazole, T-60290

$C_4H_3F_3O_2$
2-(Trifluoromethyl)propenoic acid, T-60295

$C_4H_3F_3O_4$
Trifluorobutanedioic acid, T-80269

$C_4H_3IN_2O_2$
▷ 5-Iodo-2,4(1*H*,3*H*)-pyrimidinedione, I-60062
6-Iodo-2,4-(1*H*,3*H*)-pyrimidinedione, I-70057

C_4H_3IS
3-Iodothiophene, I-60067

$C_4H_3I_3N_2$
2,4,5-Triiodo-1*H*-imidazole; 1-Me, *in* T-70276

C_4H_3N
2-Ethynyl-2*H*-azirine, E-80071
3-Ethynyl-2*H*-azirine, E-80072

C_4H_3NO
2*H*-Pyrrol-2-one, P-80228

C_4H_3NOS
2-Thiazolecarboxaldehyde, T-80170
4-Thiazolecarboxaldehyde, T-80171
5-Thiazolecarboxaldehyde, T-80172

$C_4H_3NO_2$
3-Amino-3-cyclobutene-1,2-dione, A-80065

$C_4H_3NO_3$
5-Isoxazolecarboxylic acid, I-60142

$C_4H_3N_3$
4(5)-Cyanoimidazole, *in* I-60004
4(5)-Ethynyl-1,2,3-triazole, E-80079

$C_4H_3N_3O_2$
2-Nitropyrimidine, N-60043

$C_4H_3N_3O_3$
6-Formyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione, F-60075

$C_4H_3N_3O_4$
2,3-Dinitro-1*H*-pyrrole, D-60461
2,4-Dinitro-1*H*-pyrrole, D-60462
2,5-Dinitro-1*H*-pyrrole, D-60463
3,4-Dinitro-1*H*-pyrrole, D-60464

$C_4H_3N_5$
Tetrazolo[1,5-*a*]pyrimidine, T-60176
Tetrazolo[1,5-*c*]pyrimidine, T-60177

$C_4H_3N_5O$
[1,2,4]-Triazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one, T-80214

C_4H_4
1,3-Cyclobutadiene, C-70212

C_4H_4BrNO
5-(Bromomethyl)isoxazole, B-80221

$C_4H_4BrN_3$
2-Amino-4-bromopyrimidine, A-70100
2-Amino-5-bromopyrimidine, A-70101
4-Amino-5-bromopyrimidine, A-70102
5-Amino-2-bromopyrimidine, A-70103
4-Bromo-5-methyl-1,2,3-triazine, B-80232
5-Bromo-4-methyl-1,2,3-triazine, B-80233

$C_4H_4BrN_3O_2$
4-Bromo-3(5)-nitro-1*H*-pyrazole; 1-Me, *in* B-60304

$C_4H_4Br_2$
▷ 1,4-Dibromo-2-butyne, D-70087

$C_4H_4Br_2O$
2,2-Dibromocyclopropanecarboxaldehyde, D-60092

$C_4H_4Br_2O_2$
2,2-Dibromocyclopropanecarboxylic acid, D-60093

$C_4H_4ClF_3O$
4,4,4-Trifluorobutanoic acid; Chloride, *in* T-80270

$C_4H_4ClN_3$
1-Azido-4-chloro-2-butyne, A-80195

$C_4H_4Cl_2O_2$
2,2-Dichlorocyclopropanecarboxylic acid, D-60127
Methylpropanedioic acid; Dichloride, *in* M-80149

$C_4H_4FN_3$
3-Amino-6-fluoropyridazine, A-70148

$C_4H_4F_2$
1,1-Difluoro-1,3-butadiene, D-70162
3,3-Difluorocyclobutene, D-70165

$C_4H_4F_2O_4$
2,2-Difluorobutanedioic acid, D-70163

$C_4H_4F_3NO$
2-(Trifluoromethyl)propenoic acid; Amide, *in* T-60295

$C_4H_4F_4N_2O_2$
Tetrafluorobutanedioic acid; Diamide, *in* T-80049

$C_4H_4N_2$
3,4-Diazatricyclo[3.1.0.0^{2,6}]hex-3-ene, D-70054
Methylpropanedinitrile, *in* M-80149

$C_4H_4N_2OS$
2-Thiazolecarboxaldehyde; Oxime, *in* T-80170
4-Thiazolecarboxaldehyde; Oxime, *in* T-80171
5-Thiazolecarboxaldehyde; Oxime, *in* T-80172

$C_4H_4N_2O_2$
1*H*-Imidazole-4-carboxylic acid, I-60004
5-Isoxazolecarboxylic acid; Amide, *in* I-60142
3-Nitropyrrole, N-60044
Racemic acid; Dinitrile, *in* T-70005

$C_4H_4N_2S$
4-Vinyl-1,2,3-thiadiazole, V-60014
5-Vinyl-1,2,3-thiadiazole, V-60015

$C_4H_4N_2S_2$
3-Mercapto-6(1*H*)-pyridazinethione, M-80028

$C_4H_4N_2S_3$
6-Mercapto-2,4(1*H*,3*H*)-pyrimidinedithione, M-80030

$C_4H_4N_4$
4-Amino-3-cyanopyrazole, *in* A-70189
5-Amino-4-pyrazolecarbonitrile, *in* A-70187
1*H*-Pyrazolo[5,1-*c*]-1,2,4-triazole, P-70157

$C_4H_4N_6$
4,4′-Bi-1*H*-1,2,3-triazole, B-80168
4,4′-Bi-4*H*-1,2,4-triazole, B-60189

$C_4H_4N_6O_2S$
3,4-Diazido-3,5-dihydro-thiophene 1,1-dioxide, D-80063

C_4H_4O
5-Oxabicyclo[2.1.0]pent-2-ene, O-70059

C_4H_4OS
Thiophene-3-ol, T-60212

$C_4H_4O_2$
3-Butynoic acid, B-70309
1,2-Cyclobutanedione, C-60183

$C_4H_4O_2S$
2,4(3*H*,5*H*)-Thiophenedione, T-70185

$C_4H_4O_3$
Dihydro-2,3(2*H*,3*H*)-furandione, *in* H-80227
2,4-(3*H*,5*H*)-Furandione, F-80087
Methanetricarboxaldehyde, M-80038

$C_4H_4O_3S_2$
2-Thiophenesulfonic acid, T-60213
3-Thiophenesulfonic acid, T-60214

$C_4H_4O_4$
Diformylacetic acid, D-60190
Dihydro-3-hydroxy-2,5-furandione, D-80211
1,4-Dioxane-2,6-dione, D-80500

$C_4H_4O_4S_2$
(Dimercaptomethylene)propanedioic acid, D-60395

$C_4H_4O_5$
Hydroxymethylenepropanedioic acid, H-80204

$C_4H_4Se_2$
2-Methylene-1,3-diselenole, M-70069

C_4H_5Br
1-Bromo-1,2-butadiene, B-70196
4-Bromo-1-butyne, B-70198

$C_4H_5BrN_2$
3-Bromo-1,4-dimethylpyrazole, *in* B-70250
4-Bromo-1-methyl-1*H*-imidazole, *in* B-70221
5-Bromo-1-methyl-1*H*-imidazole, *in* B-70221
3(5)-Bromo-4-methylpyrazole, B-70250
3(5)-Bromo-5(3)-methylpyrazole, B-70252
4-Bromo-3(5)-methylpyrazole, B-70251
▷ 4-Bromo-1-methylpyrazole, *in* B-80254

$C_4H_5BrN_2O$
5-Aminomethyl-3-bromoisoxazole, A-70165

$C_4H_5BrO_2$
2-Bromomethyl-2-propenoic acid, B-70249

$C_4H_5BrO_2S$
4-Bromo-2-sulfolene, *in* B-70204

C_4H_5BrS
3-Bromo-2,3-dihydrothiophene, B-70204

$C_4H_5Br_2ClO$
2,4-Dibromobutanoic acid; Chloride, *in* D-80080

C_4H_5Cl
4-Chloro-1-butyne, C-70058

$C_4H_5ClN_2$
3(5)-Chloro-5(3)-methylpyrazole, C-70109
▷ 4-Chloro-3(5)methylpyrazole, C-70108
3-Chloro-1-methylpyrazole, *in* C-70155
4-Chloro-1-methylpyrazole, *in* C-70156
5-Chloro-1-methylpyrazole, *in* C-70155

$C_4H_5ClN_4$
2,4-Diamino-5-chloropyrimidine, D-80057
▷ 2,4-Diamino-6-chloropyrimidine, D-80058

$C_4H_5ClN_4O$
2,4-Diamino-5-chloropyrimidine; 3-Oxide, *in* D-80057
2,4-Diamino-6-chloropyrimidine; 3-Oxide, *in* D-80058

C_4H_5ClO
4-Chloro-2-butyn-1-ol, C-80044

$C_4H_5Cl_2NO_2$
2-Amino-4,4-dichloro-3-butenoic acid, A-60125

$C_4H_5Cl_3O$
▷ (2,2,2-Trichloroethyl)oxirane, T-60252

$C_4H_5FO_2$
Dihydro-3-fluoro-2(3*H*)-furanone, D-80208

$C_4H_5F_3N_2O_2$
Trifluorobutanedioic acid; Diamide, *in* T-80269

$C_4H_5F_3O_2$
Trifluoroacetic acid; Et ester, *in* T-80267
4,4,4-Trifluorobutanoic acid, T-80270
3,3,3-Trifluoropropanoic acid; Me ester, *in* T-80284

$C_4H_5F_6NO$
N-Ethoxy-1,1,1,1′,1′,1′-hexafluorodimethylamine, *in* B-60180

C_4H_5I
4-Iodo-1-butyne, I-70024

$C_4H_5IN_2$
3(5)-Iodo-4-methylpyrazole, I-70048
3(5)-Iodo-5(3)-methylpyrazole, I-70050
4-Iodo-3(5)-methylpyrazole, I-70049
3-Iodo-1-methylpyrazole, *in* I-80040
4-Iodo-1-methylpyrazole, *in* I-80041
5-Iodo-1-methylpyrazole, *in* I-80040

$C_4H_5IO_2$
Dihydro-3-iodo-2(3*H*)-furanone, D-60252

C_4H_5NO
1,2-Dihydro-3*H*-pyrrol-3-one, D-70262
▷ 2-Hydroxy-3-butenenitrile, *in* P-70119
4-Oxobutanenitrile, *in* O-80068

$C_4H_5NO_2$
1-Amino-2-cyclopropene-1-carboxylic acid, A-60122
1-Aminocyclopropenecarboxylic acid, A-70126
1-Nitro-1,3-butadiene, N-60023

$C_4H_5NO_2S_2$
2-Thiophenesulfonic acid; Amide, *in* T-60213
3-Thiophenesulfonic acid; Amide, *in* T-60214

$C_4H_5NO_3$
3-Amino-2-formyl-2-propenoic acid, A-80134
2,5-Dihydro-3-nitrofuran, D-70236
2,4-(3*H*,5*H*)-Furandione; Oxime, *in* F-80087
2,3-Morpholinedione, M-80193

$C_4H_5NO_4$
3,4-Dihydroxy-2,5-pyrrolidinedione, D-80377
2-Oxo-4-oxazolidinecarboxylic acid, O-60082

C_4H_5NS
4-Mercapto-2-butenoic acid; Nitrile, *in* M-60018
3-Thiocyanato-1-propene, T-80189

$C_4H_5NS_2$
2-(Methylthio)thiazole, *in* T-60200

$C_4H_5N_3$
3-Azido-1-butyne, A-80193

$C_4H_5N_3O$
4(5)-Acetyl-1,2,3-triazole, A-80031
5-Amino-4(1*H*)-pyrimidinone, A-70196
▷ 4-Azido-2-butyn-1-ol, A-80194
1*H*-Imidazole-4-carboxylic acid; Amide, *in* I-60004
▷ 1-Methyl-2-nitroso-1*H*-imidazole, *in* N-80059

$C_4H_5N_3O_2$
▷ 3-Amino-1*H*-pyrazole-4-carboxylic acid, A-70187
3-Amino-1*H*-pyrazole-5-carboxylic acid, A-70188
4-Amino-1*H*-pyrazole-3-carboxylic acid, A-70189
4-Amino-1*H*-pyrazole-5-carboxylic acid, A-70190
5-Amino-1*H*-pyrazole-3-carboxylic acid, A-70191
5-Amino-1*H*-pyrazole-4-carboxylic acid, A-70192
3-Azido-2-propenoic acid; Me ester, *in* A-70290
6-Methyl-1,3,5-triazine-2,4(1*H*,3*H*)-dione, M-60132
1*H*-1,2,3-Triazole-4-carboxylic acid; 1-Me, *in* T-60239
1*H*-1,2,3-Triazole-4-carboxylic acid; 2-Me, *in* T-60239
1*H*-1,2,3-Triazole-4-carboxylic acid; Me ester, *in* T-60239

$C_4H_5N_3S_2$
5-Amino-2-thiazolecarbothioamide, A-60260
5-Amino-4-thiazolecarbothioamide, A-60261

C_4H_6BrN
α-Bromoisobutyronitrile, *in* B-80229

C_4H_6BrNO
3-Bromo-2-pyrrolidinone, B-80258

$C_4H_6BrNO_4$
2-Amino-3-bromobutanedioic acid, A-70098

$C_4H_6Br_2O$
2-Bromo-2-methylpropanoic acid; Bromide, *in* B-80229

$C_4H_6Br_2O_2$
2,4-Dibromobutanoic acid, D-80080

$C_4H_6ClF_2NO_2$
2-Amino-4-chloro-4,4-difluorobutanoic acid, A-60107

$C_4H_6ClNO_2$
1-Chloro-1-nitrocyclobutane, C-70130

$C_4H_6ClNO_4$
2-Amino-3-chlorobutanedioic acid, A-70121

$C_4H_6Cl_2$
3-Chloro-2-chloromethyl-1-propene, C-70061

$C_4H_6F_3NO$
4,4,4-Trifluorobutanoic acid; Amide, *in* T-80270

$C_4H_6I_2$
▷ 3-Iodo-2-(iodomethyl)-1-propene, I-60047

$C_4H_6N_2$
3-Aminopyrrole, A-80143
1,4-Dihydropyrimidine, D-70255

$C_4H_6N_2O$
3-Amino-4-methylisoxazole, A-80106
4-Amino-3-methylisoxazole, A-80107
4-Amino-5-methylisoxazole, A-80108
5-Amino-4-methylisoxazole, A-80109
4,5-Dihydro-3(2*H*)-pyridazinone, D-60272
3,4-Dihydro-2(1*H*)-pyrimidinone, D-60273
5,6-Dihydro-4(1*H*)-pyrimidinone, D-60274
4(5)-Methoxyimidazole, M-80044

$C_4H_6N_2OS$
2-Thioxo-4-imidazolidinone; 1-*N*-Me, *in* T-70188
2-Thioxo-4-imidazolidinone; 3-*N*-Me, *in* T-70188

$C_4H_6N_2O_2$
1,3-Diazetidine-2,4-dione; 1,3-Di-Me, *in* D-60057
Dihydro-4,6-(1*H*,5*H*)-pyrimidinedione, D-70256
Dimethyl *N*-cyanoimidocarbonate, D-70390

$C_4H_6N_2O_3$
3-Methoxy-4-methyl-1,2,4-oxadiazolidin-5(4*H*)-one, *in* O-70060
1,2,4-Oxadiazolidine-3,5-dione; 2,4-Di-Me, *in* O-70060
1,2,4-Oxadiazolidine-3,5-dione; 4-Et, *in* O-70060
2-Oxo-4-imidazolidinecarboxylic acid, O-60074

$C_4H_6N_2S$
2-(Methylthio)-1*H*-imidazole, *in* D-80215

$C_4H_6N_2S_2$
2,5-Dihydro-4,6-pyrimidinedithiol, D-70257

$C_4H_6N_2S_3$
2,5-Bis(methylthio)-1,3,4-thiadiazole, *in* M-70031
3-Methyl-5-(methylthio)-1,3,4-thiadiazole-2(3*H*)-thione, *in* M-70031

$C_4H_6N_4$
3-Amino-1,2,4-triazine; *N*-Me, *in* A-70203

$C_4H_6N_4O$
2-Amino-4-methoxy-1,3,5-triazine, *in* A-80149
3-Amino-1*H*-pyrazole-4-carboxylic acid; Amide, *in* A-70187
4-Amino-1*H*-pyrazole-3-carboxylic acid; Amide, *in* A-70189
4-Amino-1*H*-pyrazole-5-carboxylic acid; *N*(1)-Me, Amide, *in* A-70190
4-Amino-1,3,5-triazin-2(1*H*)-one; 4-*N*-Me, *in* A-80149
2,6-Diamino-4(1*H*)-pyrimidinone, D-70043
1*H*-1,2,3-Triazole-4-carboxylic acid; 1-Me, amide, *in* T-60239

$C_4H_6N_4O_2$
3,6-Dimethoxy-1,2,4,5-tetrazine, *in* D-70268
Tetrahydroimidazo[4,5-*d*]imidazole-2,5(1*H*,3*H*)-dione, T-70066

C_4H_6OS
Dihydro-2(3*H*)-furanthione, D-70210

$C_4H_6O_2$
▷ Methyl acrylate, *in* P-70121
2-Methylene-1,3-dioxolane, M-60075
4-Methylene-1,3-dioxolane, M-60076
2-Oxetanecarboxaldehyde, O-80053
2-Oxobutanal, O-80067

$C_4H_6O_2S$
4-Mercapto-2-butenoic acid, M-60018
3-Oxobutanethioic acid, O-70080

$C_4H_6O_3$
Dihydro-3-hydroxy-2(3*H*)-furanone, D-80212
Dihydro-4-hydroxy-2(3*H*)-furanone, D-60242
4,5-Dihydro-3-hydroxy-2(3*H*)-furanone, *in* D-60313
2-Formylpropanoic acid, F-70039
4-Hydroxy-2-butenoic acid, H-80134
1-Hydroxycyclopropanecarboxylic acid, H-60117
Methylene-1,3,5-trioxane, M-60081
3-Methyloxiranecarboxylic acid, M-80127
▷ 4-Oxobutanoic acid, O-80068
3-Oxopropanoic acid; Me ester, *in* O-60090

$C_4H_6O_4$
3-Hydroxy-2-oxobutanoic acid, H-80226
4-Hydroxy-2-oxobutanoic acid, H-80227
▷ Methylpropanedioic acid, M-80149

$C_4H_6O_5$
Dimethyl dicarbonate, *in* D-70111
Glycolloglycollic acid, G-80030

$C_4H_6O_6$
Tartaric acid, T-70005

C_4H_6S
2,5-Dihydrothiophene, D-70270

$C_4H_6S_2$
2-Butyne-1,4-dithiol, B-70308

$C_4H_6S_2Se$
1,3-Dithiane-2-selone, D-70507

$C_4H_6S_4$
Ethanebis(dithioic)acid; Di-Me ester, *in* E-60040

$C_4H_6Se_2$
2-Methyl-1,3-diselenole, M-80070

C_4H_7Br
1-Bromo-1-methylcyclopropane, B-70242

C_4H_7BrO
4-Bromobutanal, B-70197

$C_4H_7BrO_2$
▷ 2-Bromo-2-methylpropanoic acid, B-80229

$C_4H_7Br_2NO$
2,4-Dibromobutanoic acid; Amide, *in* D-80080

C_4H_7Cl
3-Chloro-1-butene, C-80042

$C_4H_7ClFNO_2$
2-Amino-4-chloro-4-fluorobutanoic acid, A-60108

C_4H_7ClOS
Carbonochloridothioic acid; *O*-Isopropyl, *in* C-60013
Carbonochloridothioic acid; *O*-Propyl, *in* C-60013
▷ Carbonochloridothioic acid; *S*-Propyl, *in* C-60013

$C_4H_7ClO_3$
3-Chloro-2-hydroxypropanoic acid; Me ester, *in* C-70072

$C_4H_7Cl_3$
1,3-Dichloro-2-(chloromethyl)propane, D-70118

$C_4H_7F_2NO_2$
2-Amino-3,3-difluorobutanoic acid, A-60133
3-Amino-4,4-difluorobutanoic acid, A-60134

$C_4H_7F_3OS$
Trifluoromethanesulfenic acid; Isopropyl ester, *in* T-60279

C_4H_7IO
2-Iodobutanal, I-60040
3-Iodo-2-butanone, I-60041
2-Iodomethyl-3-methyloxirane, I-80034
2-Iodo-2-methylpropanal, I-60051
Tetrahydro-2-iodofuran, T-80069

$C_4H_7I_3$
1,3-Diiodo-2-(iodomethyl)propane, D-70358

C_4H_7N
3-Butyn-1-amine, B-80294
3,4-Dihydro-2*H*-pyrrole, D-80247
2-Propyn-1-amine; *N*-Me, *in* P-60184

C_4H_7NO
▷ 2-Pyrrolidinone, P-70188

C_4H_7NOS
Tetrahydro-2*H*-1,2-thiazin-3-one, T-60095
Tetrahydro-2*H*-1,3-thiazin-2-one, T-60096
3-Thiomorpholinone, T-80190

$C_4H_7NO_2$
3-Aminodihydro-2(3*H*)-furanone, A-60138
4-Aminodihydro-2(3*H*)-furanone, *in* A-80081
2-Azetidinecarboxylic acid, A-70284
5-Methyl-2-oxazolidinone, M-60107
3-Morpholinone, M-60147
Nitrocyclobutane, N-60024
2-Oxobutanal; 1-Oxime, *in* O-80067

$C_4H_7NO_2S$
3-Thiomorpholinone; S-Oxide, *in* T-80190

$C_4H_7NO_3$
1-Nitro-2-butanone, N-70043
3-Nitro-2-butanone, N-70044
4-Nitro-2-butanone, N-70045
4-Oxobutanoic acid; Oxime, *in* O-80068

$C_4H_7NO_3S$
3-Thiomorpholinone; S-Dioxide, *in* T-80190

C_4H_7NS
2-Propenethioamide; *N*-Me, *in* P-70120
2-Pyrrolidinethione, P-70186

$C_4H_7NS_2$
4,5-Dihydro-2-(methylthio)thiazole, *in* T-60197
Tetrahydro-2*H*-1,3-thiazine-2-thione, T-60094
2-Thiazoledinethione; *N*-Me, *in* T-60197

$C_4H_7N_3O$
4-Azidobutanal, A-70286
4,5-Dihydro-5,5-dimethyl-3*H*-1,2,4-triazol-3-one, D-80196

$C_4H_7N_3O_3$
Biuret; *N*-Ac, *in* B-60190

$C_4H_7N_5$
2,4-Diamino-6-methyl-1,3,5-triazine, D-60040
2,4,6-Triaminopyrimidine, T-80208

$C_4H_7N_5O$
5-Acetamido-2-methyl-2*H*-tetrazole, *in* A-70202
2,4-Diamino-6-methyl-1,3,5-triazine; N^3-Oxide, *in* D-60040
2,4-Diamino-6-methyl-1,3,5-triazine; N^5-Oxide, *in* D-60040

C_4H_8BrNO
2-Bromo-2-methylpropanoic acid; Amide, *in* B-80229

$C_4H_8BrNO_2$
2-Amino-3-bromobutanoic acid, A-60097
2-Amino-4-bromobutanoic acid, A-60098
4-Amino-2-bromobutanoic acid, A-60099

C_4H_8ClN
4-Chloro-2-buten-1-amine, C-50094

$C_4H_8ClNO_2$
2-Amino-3-chlorobutanoic acid, A-60103
2-Amino-4-chlorobutanoic acid, A-60104
4-Amino-2-chlorobutanoic acid, A-60105
4-Amino-3-chlorobutanoic acid, A-60106

$C_4H_8FNO_2$
2-Amino-3-fluorobutanoic acid, A-60154
2-Amino-4-fluorobutanoic acid, A-60155
3-Amino-4-fluorobutanoic acid, A-60156
4-Amino-2-fluorobutanoic acid, A-60157
4-Amino-3-fluorobutanoic acid, A-60158

$C_4H_8I_2O$
1,1′-Oxybis[2-iodoethane], O-60096

$C_4H_8N_2O$
2-Imidazolidinone; 1-Me, *in* I-70005
Piperazinone, P-70101
Tetrahydro-2(1*H*)-pyrimidinone, T-60088
Tetrahydro-4(1*H*)-pyrimidinone, T-60089

$C_4H_8N_2O_2$
Acetamidoxime; *O*-Ac, *in* A-60016
4-Amino-5-methyl-3-isoxazolidinone, A-60221
Methylpropanedioic acid; Diamide, *in* M-80149

$C_4H_8N_2O_4$
L-Threaric acid; Diamide, *in* T-70005

$C_4H_8N_4O_2$
1,4-Dihydro-3,6-dimethoxy-1,2,4,5-tetrazine, D-70192
▷ Hexahydropyrimidine; *N,N′*-Dinitroso, *in* H-60056
Tetrahydro-1,3,5,7-tetrazocine-2,6(1*H*,3*H*)-dione, T-70098

$C_4H_8N_4O_4$
▷ Hexahydropyrimidine; *N,N′*-Dinitro, *in* H-60056

C_4H_8O
▷ 2-Ethyloxirane, E-70047

C_4H_8OS
(Ethylthio)acetaldehyde, *in* M-80017
3-Mercaptocyclobutanol, M-60019
Tetrahydro-3-furanthiol, T-80063

$C_4H_8O_2$
3-Butene-1,2-diol, B-70291
2-Hydroxybutanal, H-70112
▷ 2-Methyl-1,3-dioxolane, M-60063
3-Methyloxiranemethanol, M-80128
2-Oxetanemethanol, O-80054
3-Oxetanemethanol, O-80055

$C_4H_8O_2S$
3-Mercaptobutanoic acid, M-70023
2-(Methylthio)propanoic acid, *in* M-60027

$C_4H_8O_3$
1,3-Dioxolane-2-methanol, D-70468

$C_4H_8O_4$
2,3-Dihydroxybutanoic acid, D-60312
3,4-Dihydroxybutanoic acid, D-60313

$C_4H_8O_5S$
Sulfoacetic acid; Carboxy-Et ester, *in* S-80050

$C_4H_8S_2$
2-Butene-1,4-dithiol, B-70292
1,1-Cyclobutanedithiol, C-70215
1,3-Cyclobutanedithiol, C-60184
2-Methylene-1,3-propanedithiol, M-70076

$C_4H_8S_2^{2\oplus}$
1,4-Dithioniabicyclo[2.2.0]hexane, D-70527

$C_4H_9BF_4S_3$
Tris(methylthio)methylium(1+); Tetrafluoroborate, *in* T-80367

C_4H_9ClOS
tert-Butylsulfinic acid; Chloride, *in* B-80293

$C_4H_9ClO_2$
2-Chloro-1,4-butanediol, C-80040

$C_4H_9F_3O_3SSi$
Trifluoromethanesulfonic acid; Trimethylsilyl ester, *in* T-70241

C_4H_9IO
tert-Butyl hypoiodite, B-80287

C_4H_9N
▷ 2-Buten-1-amine, B-80278

C_4H_9NO
▷ Acetamide; *N*-Di-Me, *in* A-70019
4-Aminobutanal, A-80064
3-Pyrrolidinol, P-70187

$C_4H_9NO_3$
2-Amino-4-hydroxybutanoic acid, A-70156
3-Amino-2-hydroxybutanoic acid, A-60183
3-Amino-4-hydroxybutanoic acid, A-80081
Threonine, T-60217

C_4H_9NS
▷ Tetrahydro-2*H*-1,3-thiazine, T-60093

$C_4H_9N_3O$
1-Azido-1-methoxypropane, *in* A-80204

$C_4H_9N_3O_3$
3-Amino-2-ureidopropanoic acid, A-60268

$C_4H_9N_5$
N-(1,4-Dihydro-1,4-dimethyl-5*H*-tetrazol-5-ylidene)methanamine, *in* A-70202

$C_4H_9S_3^{\oplus}$
Tris(methylthio)methylium(1+), T-80367

$C_4H_{10}NO_6P$
O-Phosphohomoserine, *in* A-70156

$C_4H_{10}N_2$
Hexahydropyrimidine, H-60056

$C_4H_{10}N_2O$
Tetrahydro-3,4-furandiamine, T-70062

$C_4H_{10}N_4$
Octahydroimidazo[4,5-*d*]imidazole, O-70015

$C_4H_{10}O_2$
▷ 1-Methoxy-2-propanol, *in* P-70118
2-Methyl-1,3-propanediol, M-60120

$C_4H_{10}O_2S$
tert-Butylsulfinic acid, B-80293

$C_4H_{10}O_3$
▷ 1-Ethoxy-1-hydroperoxyethane, E-60044
2-Hydroxymethyl-1,3-propanediol, H-80212

$C_4H_{10}S_2$
1,3-Butanedithiol, B-60339
2,2-Butanedithiol, B-60340
2-Methyl-1,3-propanedithiol, M-60121

$C_4H_{12}N_4$
Octahydro-1,2,5,6-tetrazocine, O-60020
▷ 1,1,4,4-Tetramethyl-2-tetrazene, T-80153

$C_4H_{13}N_3O$
2-[(2-Hydrazinoethyl)amino]ethanol, H-60091

C_4N_6
3,6-Dicyano-1,2,4,5-tetrazine, *in* T-80163

$C_4N_6S_2$
Bis[1,2,5-thiadiazolo][3,4-*b*:3′,4′-*e*]pyrazine, B-70161

C_5BrF_4N
2-Bromo-3,4,5,6-tetrafluoropyridine, B-60326
4-Bromo-2,3,5,6-tetrafluoropyridine, B-60328

C_5BrF_5N
3-Bromo-2,4,5,6-tetrafluoropyridine, B-60327

C_5F_6
1,2,3,4,5,5-Hexafluoro-1,3-cyclopentadiene, H-60044

$C_5F_{10}N_2O_2$
2,2,3,3,4,4,5,5,6,6-Decafluoropiperidine; *N*-Nitro, *in* D-60006

$C_5F_{11}N$
Undecafluoropiperidine, U-60002

$C_5F_{12}S_4$
Tetrakis(trifluoromethylthio)methane, T-80133

$C_5HF_{10}N$
2,2,3,3,4,4,5,5,6,6-Decafluoropiperidine, D-60006

$C_5H_2Cl_2N_2O_2$
2,3-Dichloro-5-nitropyridine, D-60140
2,4-Dichloro-3-nitropyridine, D-60141
2,4-Dichloro-5-nitropyridine, D-60142
2,5-Dichloro-3-nitropyridine, D-60143
2,6-Dichloro-3-nitropyridine, D-60144
2,6-Dichloro-4-nitropyridine, D-60145
3,4-Dichloro-5-nitropyridine, D-60146
3,5-Dichloro-4-nitropyridine, D-60147

$C_5H_2Cl_2N_2O_3$
2,6-Dichloro-4-nitropyridine; 1-Oxide, *in* D-60145
3,5-Dichloro-4-nitropyridine; 1-Oxide, *in* D-60147

$C_5H_2Cl_3N$
▷ 2,4,6-Trichloropyridine, T-60255

$C_5H_2Cl_3NOS$
2-(Trichloroacetyl)thiazole, T-80222

$C_5H_2F_4N_2$
4-Amino-2,3,5,6-tetrafluoropyridine, A-60257

$C_5H_2F_6O$
4,4,4-Trifluoro-3-(trifluoromethyl)-2-butenal, T-60309
1,1,1-Trifluoro-2-(trifluoromethyl)-3-butyn-2-ol, T-60310

C_5H_2INS
2-Cyano-3-iodothiophene, *in* I-60075
2-Cyano-4-iodothiophene, *in* I-60076
2-Cyano-5-iodothiophene, *in* I-60078
3-Cyano-2-iodothiophene, *in* I-60074
3-Cyano-4-iodothiophene, *in* I-60077
4-Cyano-2-iodothiophene, *in* I-60079

$C_5H_2S_4$
Thieno[2,3-*d*]-1,3-dithiole-2-thione, T-80175

C_5H_3BrClN
3-Bromo-5-chloropyridine, B-60223
4-Bromo-3-chloropyridine, B-60224

C_5H_3BrFN
2-Bromo-3-fluoropyridine, B-70213
2-Bromo-5-fluoropyridine, B-60252
3-Bromo-2-fluoropyridine, B-60253
3-Bromo-4-fluoropyridine, B-70214
3-Bromo-5-fluoropyridine, B-60254
4-Bromo-3-fluoropyridine, B-60255
5-Bromo-2-fluoropyridine, B-60256

C_5H_3BrIN
2-Bromo-4-iodopyridine, B-60280
2-Bromo-5-iodopyridine, B-60281
3-Bromo-4-iodopyridine, B-60282
3-Bromo-5-iodopyridine, B-60283
4-Bromo-2-iodopyridine, B-60284
4-Bromo-3-iodopyridine, B-60285
5-Bromo-2-iodopyridine, B-60286

$C_5H_3BrO_2$
3-Bromo-2-furancarboxaldehyde, B-60257
4-Bromo-2-furancarboxaldehyde, B-60258
5-Bromo-2-furancarboxaldehyde, B-60259

$C_5H_3Br_2NO$
4,6-Dibromo-2(1*H*)pyridone, D-80100

C_5H_3ClFN
2-Chloro-3-fluoropyridine, C-60081
2-Chloro-4-fluoropyridine, C-60082
2-Chloro-5-fluoropyridine, C-60083
2-Chloro-6-fluoropyridine, C-60084
3-Chloro-2-fluoropyridine, C-60085
4-Chloro-2-fluoropyridine, C-60086
4-Chloro-3-fluoropyridine, C-60087
5-Chloro-2-fluoropyridine, C-60088

C_5H_3ClFNO
2-Chloro-3-fluoropyridine; *N*-Oxide, *in* C-60081

C_5H_3ClIN
2-Chloro-3-iodopyridine, C-60107
2-Chloro-4-iodopyridine, C-60108
2-Chloro-5-iodopyridine, C-60109
3-Chloro-2-iodopyridine, C-60110
3-Chloro-5-iodopyridine, C-60111
4-Chloro-2-iodopyridine, C-60112
4-Chloro-3-iodopyridine, C-60113

C_5H_3FIN
2-Fluoro-3-iodopyridine, F-80048
2-Fluoro-4-iodopyridine, F-60045
3-Fluoro-4-iodopyridine, F-60046

C_5H_3IOS
2-Iodo-3-thiophenecarboxaldehyde, I-60068
3-Iodo-2-thiophenecarboxaldehyde, I-60069
4-Iodo-2-thiophenecarboxaldehyde, I-60070
4-Iodo-3-thiophenecarboxaldehyde, I-60071
5-Iodo-2-thiophenecarboxaldehyde, I-60072
5-Iodo-3-thiophenecarboxaldehyde, I-60073

$C_5H_3IO_2S$
2-Iodo-3-thiophenecarboxylic acid, I-60074
3-Iodo-2-thiophenecarboxylic acid, I-60075
4-Iodo-2-thiophenecarboxylic acid, I-60076
4-Iodo-3-thiophenecarboxylic acid, I-60077
5-Iodo-2-thiophenecarboxylic acid, I-60078
5-Iodo-3-thiophenecarboxylic acid, I-60079

C_5H_3N
3,4-Pyridyne, P-80224

$C_5H_3NO_4S$
4-Nitro-2-thiophenecarboxylic acid, N-80061
5-Nitro-2-thiophenecarboxylic acid, N-80062

C_5H_3NS
2-Ethynylthiazole, E-60061
4-Ethynylthiazole, E-60062

$C_5H_3N_5O_8$
▷ 1-Methyl-2,3,4,5-tetranitro-1*H*-pyrrole, *in* T-60160

C_5H_4BrNO
▷ 2-Bromo-3-hydroxypyridine, B-60275
2-Bromo-5-hydroxypyridine, B-60276
3-Bromo-5-hydroxypyridine, B-60277
4-Bromo-3-hydroxypyridine, B-60278

$C_5H_4BrNO_2$
2-Bromo-3-hydroxypyridine; *N*-Oxide, *in* B-60275

C_5H_4BrNS
3-Bromo-2(1*H*)-pyridinethione, B-60315
3-Bromo-4(1*H*)-pyridinethione, B-60316
5-Bromo-2(1*H*)-pyridinethione, B-60317
6-Bromo-2(1*H*)-pyridinethione, B-80256

$C_5H_4BrN_5O$
8-Bromoguanine, B-80205

C_5H_4ClNO
▷ 2-Chloro-3-hydroxypyridine, C-60100
2-Chloro-5-hydroxypyridine, C-60101
3-Chloro-5-hydroxypyridine, C-60102

$C_5H_4ClNO_2$
4-Chloro-6-hydroxy-2(1*H*)-pyridinone, C-70073
6-Chloro-4-hydroxy-2(1*H*)pyridinone, C-70074
▷ 5-Methyl-4-isoxazolecarboxylic acid; Chloride, *in* M-80117

$C_5H_4ClNO_2S$
2-Pyridinesulfonic acid; Chloride, *in* P-70171

C_5H_4ClNS
3-Chloro-2(1*H*)-pyridinethione, C-60129

$C_5H_4ClN_5$
▷ 2-Amino-6-chloro-1*H*-purine, A-60116
2-Chloro-6-aminopurine, C-70039

$C_5H_4ClN_5O$
8-Chloroguanine, C-80057

$C_5H_4Cl_4$
1-Chloro-1-(trichlorovinyl)cyclopropane, C-60138

$C_5H_4FN_5$
8-Amino-6-fluoro-9*H*-purine, A-60163

C_5H_4INO
3-Hydroxy-2-iodopyridine, H-60160

C_5H_4INOS
2-Iodo-3-thiophenecarboxaldehyde; Oxime, *in* I-60068
3-Iodo-2-thiophenecarboxaldehyde; Oxime, *in* I-60069
4-Iodo-2-thiophenecarboxaldehyde; Oxime, *in* I-60070
4-Iodo-3-thiophenecarboxaldehyde; Oxime, *in* I-60071
5-Iodo-2-thiophenecarboxaldehyde; Oxime, *in* I-60072
5-Iodo-3-thiophenecarboxaldehyde; Oxime, *in* I-60073
2-Iodo-3-thiophenecarboxylic acid; Amide, *in* I-60074
3-Iodo-2-thiophenecarboxylic acid; Amide, *in* I-60075
4-Iodo-2-thiophenecarboxylic acid; Amide, *in* I-60076

4-Iodo-3-thiophenecarboxylic acid; Amide, *in* I-60077
5-Iodo-2-thiophenecarboxylic acid; Amide, *in* I-60078
5-Iodo-3-thiophenecarboxylic acid; Amide, *in* I-60079

$C_5H_4IN_5O$
8-Iodoguanine, I-80031

$C_5H_4N_2$
1,1-Dicyanocyclopropane, *in* C-80196

$C_5H_4N_2O_2$
Methyl dicyanoacetate, *in* D-70149

$C_5H_4N_2O_3$
3-Nitro-4(1*H*)-pyridone, N-70063
1,2,3,4-Tetrahydro-2,4-dioxo-5-pyrimidinecarboxaldehyde, T-60064

$C_5H_4N_2O_4$
1*H*-Pyrazole-4,5-dicarboxylic acid, P-80199

$C_5H_4N_2S$
▷ 2-Thiocyanato-1*H*-pyrrole, T-60209

$C_5H_4N_4$
1*H*-Pyrazolo[3,4-*d*]pyrimidine, P-70156
Pyrazolo[1,5-*b*][1,2,4]triazine, P-60207
[1,2,4]Triazolo[1,5-*b*]pyridazine, T-60240
[1,2,4]Triazolo[1,5-*a*]pyrimidine, T-60242
1,2,4-Triazolo[4,3-*c*]pyrimidine, T-60243

$C_5H_4N_4O$
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazin-6-one, D-60248
2*H*-Imidazo[4,5-*b*]pyrazin-2-one, I-60006
Imidazo[2,1-*c*][1,2,4]triazin-4(1*H*)-one, I-80007
Pyrazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one, P-80201

$C_5H_4N_4O_2$
1*H*-Pyrazolo[3,4-*d*]pyrimidine-4,6(5*H*,7*H*)-dione, P-60202

$C_5H_4N_4O_6$
▷ 1-Methyl-2,3,4-trinitro-1*H*-pyrrole, *in* T-60373
▷ 1-Methyl-2,3,5-trinitro-1*H*-pyrrole, *in* T-60374

$C_5H_4N_4S$
1,3-Dihydro-2*H*-imidazo[4,5-*b*]pyrazine-2-thione, D-60247
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazine-6-thione, D-70215
▷ 1,7-Dihydro-6*H*-purine-6-thione, D-60270

C_5H_4OS
▷ 2-Thiophenecarboxaldehyde, T-70183

$C_5H_4OS_4$
5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-one, D-80205

$C_5H_4O_2$
3-Methyl-3-cyclobutene-1,2-dione, M-80062

$C_5H_4O_2S_2$
3-Mercapto-2-thiophenecarboxylic acid, M-80031
4-Mercapto-3-thiophenecarboxylic acid, M-80032

$C_5H_4O_3$
3-Oxabicyclo[3.1.0]hexane-2,4-dione, *in* C-70248

$C_5H_4S_5$
5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-thione, D-80206

$C_5H_5BF_5N$
1-Fluoropyridinium; Tetrafluoroborate, *in* F-60066

$C_5H_5BrN_2$
4-Bromo-6-methylpyrimidine, B-80230
5-Bromo-4-methylpyrimidine, B-80231

$C_5H_5BrN_2O$
2-Amino-5-bromo-3-hydroxypyridine, A-60101

$C_5H_5BrO_5$
(3-Bromo-2-oxopropylidene)propanedioic acid, B-70262

$C_5H_5Br_2NO$
2,6-Dibromo-4(1*H*)-pyridone, D-80099

C_5H_5Cl
1-Chloro-1-ethynylcyclopropane, C-60068

$C_5H_5ClFNO_4$
1-Fluoropyridinium; Perchlorate, *in* F-60066

$C_5H_5ClN_2$
2-Chloro-3-methylpyrazine, C-70105
2-Chloro-5-methylpyrazine, C-70106
2-Chloro-6-methylpyrazine, C-70107
3-Chloro-4-methylpyridazine, C-70110
3-Chloro-5-methylpyridazine, C-70111
3-Chloro-6-methylpyridazine, C-70112
4-Chloro-3-methylpyridazine, C-80078
4-Chloro-5-methylpyridazine, C-80079
2-Chloro-4-methylpyrimidine, C-70113
2-Chloro-5-methylpyrimidine, C-70114
4-Chloro-2-methylpyrimidine, C-70115
4-Chloro-5-methylpyrimidine, C-70116
4-Chloro-6-methylpyrimidine, C-70117
5-Chloro-2-methylpyrimidine, C-70118
5-Chloro-4-methylpyrimidine, C-70119

$C_5H_5ClN_2O$
2-Amino-5-chloro-3-hydroxypyridine, A-60111
▷ 2-Chloro-3-methylpyrazine; 1-Oxide, *in* C-70105
2-Chloro-6-methylpyrazine; 4-Oxide, *in* C-70107
3-Chloro-2-methylpyrazine 1-oxide, *in* C-70105
3-Chloro-4-methylpyridazine; 1-Oxide, *in* C-70110
3-Chloro-5-methylpyridazine; 1-Oxide, *in* C-70111
3-Chloro-6-methylpyridazine; 1-Oxide, *in* C-70112
4-Chloro-3-methylpyridazine; 1-Oxide, *in* C-80078
4-Chloro-5-methylpyridazine; 1-Oxide, *in* C-80079
4-Chloro-6-methylpyrimidine; 1-Oxide, *in* C-70117

C_5H_5ClO
2-Chloro-2-cyclopenten-1-one, C-60051
5-Chloro-2-cyclopenten-1-one, C-70063

$C_5H_5Cl_2F_3O_2$
2,2-Dichloro-3,3,3-trifluoro-1-propanol; Ac, *in* D-60161

$C_5H_5FN^{\oplus}$
1-Fluoropyridinium, F-60066

$C_5H_5F_3O_2$
Dihydro-4-(trifluoromethyl)-2(3*H*)-furanone, D-60299
Dihydro-5-(trifluoromethyl)-2(3*H*)-furanone, D-60300
▷ 2-(Trifluoromethyl)propenoic acid; Me ester, *in* T-60295

$C_5H_5F_7NSb$
1-Fluoropyridinium; Hexafluoroantimonate, *in* F-60066

C_5H_5I
5-Iodo-1-penten-4-yne, I-70053

$C_5H_5IN_2$
2-Amino-3-iodopyridine, A-80088
2-Amino-4-iodopyridine, A-80089
2-Amino-5-iodopyridine, A-80090
2-Amino-6-iodopyridine, A-80091
3-Amino-5-iodopyridine, A-80092
4-Amino-2-iodopyridine, A-80093
4-Amino-3-iodopyridine, A-80094
5-Amino-2-iodopyridine, A-80095

$C_5H_5IN_2O$
4-Amino-2-iodopyridine; N-oxide, *in* A-80093

$C_5H_5I_3N_2$
2,4,5-Triiodo-1*H*-imidazole; 1-Et, *in* T-70276

C_5H_5N
1-Cyanobicyclo[1.1.0]butane, *in* B-70094

C_5H_5NO
3-Formyl-2-butenenitrile, *in* M-70103
1*H*-Pyrrole-3-carboxaldehyde, P-70182

C_5H_5NOS
5-Acetylthiazole, A-80029
▷ 1-Hydroxy-2(1*H*)-pyridinethione, H-70217
3-Hydroxy-2(1*H*)-pyridinethione, H-60222
2-Pyridinethiol *N*-oxide, *in* P-60224
▷ 2(1*H*)-Pyridinethione; 1-Hydroxy, *in* P-60224
4(1*H*)-Pyridinethione; 1-Hydroxy, *in* P-60225
2-Pyrrolethiolcarboxylic acid, P-80226
2-Thiophenecarboxaldehyde; Oxime, *in* T-70183

C_5H_5NOSe
2(1*H*)-Pyridineselone; *N*-Oxide, *in* P-70170

$C_5H_5NO_2$
1-Cyanocyclopropanecarboxylic acid, *in* C-80196
2,3-Dihydro-3-oxo-1*H*-pyrrole-1-carboxaldehyde, *in* D-70262
3-Hydroxy-2(1*H*)-pyridinone, H-60223
3-Hydroxy-4(1*H*)-pyridinone, H-60227
4-Hydroxy-2(1*H*)-pyridinone, H-60224
5-Hydroxy-2(1*H*)-pyridinone, H-60225
6-Hydroxy-2(1*H*)-pyridinone, H-60226

$C_5H_5NO_2S$
2-Pyridinesulfinic acid, P-80208
4-Pyridinesulfinic acid, P-80209

$C_5H_5NO_3$
4,6-Dihydroxy-2(1*H*)-pyridinone, D-70341
3-Hydroxy-1*H*-pyrrole-2-carboxylic acid, H-80248
4-Hydroxy-1*H*-pyrrole-2-carboxylic acid, H-80249
4-Hydroxy-1*H*-pyrrole-3-carboxylic acid, H-80250
5-Isoxazolecarboxylic acid; Me ester, *in* I-60142
5-Methyl-4-isoxazolecarboxylic acid, M-80117

$C_5H_5NO_3S$
2-Pyridinesulfonic acid, P-70171

C_5H_5NS
2-Pyridinethiol, P-60223
▷ 2(1*H*)-Pyridinethione, P-60224
▷ 4(1*H*)-Pyridinethione, P-60225
1,4-Thiazepine, T-60196
1-Thiocyano-1,3-butadiene, T-60210

$C_5H_5NS_2$
4-Mercapto-2(1*H*)-pyridinethione, M-80029
2,3-Pyridinedithiol, P-60218
2,4-Pyridinedithiol, P-60219
2,5-Pyridinedithiol, P-60220
3,4-Pyridinedithiol, P-60221
3,5-Pyridinedithiol, P-60222

C_5H_5NSe
2(1*H*)-Pyridineselone, P-70170

$C_5H_5N_3O_2$
N-(1,4-Dihydro-4-oxo-5-pyrimidinyl)formamide, *in* A-70196
4-Methyl-5-nitropyrimidine, M-60104

$C_5H_5N_3O_4$
1-Methyl-2,3-dinitro-1*H*-pyrrole, *in* D-60461
1-Methyl-2,4-dinitro-1*H*-pyrrole, *in* D-60462
1-Methyl-2,5-dinitro-1*H*-pyrrole, *in* D-60463
1-Methyl-3,4-dinitro-1*H*-pyrrole, *in* D-60464

$C_5H_5N_5$
▷ 2-Aminopurine, A-60243
8-Aminopurine, A-60244
9-Aminopurine, A-60245

$C_5H_5N_5O$
6-Amino-1,3-dihydro-2*H*-purin-2-one, A-60144
5-Aminopyrazolo[4,3-*d*]pyrimidin-7(1*H*,6*H*)-one, A-60246
[1,2,4]-Triazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one; 1-Me, *in* T-80214
[1,2,4]-Triazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one; 2-Me, *in* T-80214

$C_5H_5N_5OS$
2-Amino-1,7,8,9-tetrahydro-2-thioxo-6*H*-purin-6-one, A-80145

C_5H_6
Ethylnylcyclopropane, E-70045
Tricyclo[1.1.1.0^{1,3}]pentane, T-80244
Tricyclo[2.1.0.0^{1,3}]pentane, T-70231
3-Vinylcyclopropene, V-60012

$C_5H_6BrN_3$
5-Bromo-4,6-dimethyl-1,2,3-triazine, B-80201

$C_5H_6Br_2Cl_2$
1,1-Dibromo-2,2-bis(chloromethyl)cyclopropane, D-80079

$C_5H_6Br_2O$
4,4-Dibromo-3-methyl-3-buten-2-one, D-70094

$C_5H_6Br_2O_2$
2,2-Dibromocyclopropanecarboxylic acid; Me ester, *in* D-60093

$C_5H_6ClN_3$
5-Chloro-4,6-dimethyl-1,2,3-triazine, C-80052

$C_5H_6ClN_3O_2$
2-Chloro-4,6-dimethoxy-1,3,5-triazine, *in* C-80115

$C_5H_6Cl_2O_2$
2,2-Dichlorocyclopropanecarboxylic acid; Me ester, *in* D-60127

$C_5H_6CrFNO_3$
▷ Pyridinium fluorochromate, P-80210

$C_5H_6F_2O_2$
3,3-Difluorocyclobutanecarboxylic acid, D-70164

$C_5H_6I_2$
1,3-Diiodobicyclo[1.1.1]pentane, D-70357

$C_5H_6N_2$
4(5)-Vinylimidazole, V-70012

$C_5H_6N_2O$
2-Amino-3-hydroxypyridine, A-60200
2-Amino-5-hydroxypyridine, A-60201
4-Amino-3-hydroxypyridine, A-60202
5-Amino-3-hydroxypyridine, A-60203
1-Amino-2(1*H*)-pyridinone, A-60248
2-Amino-4(1*H*)-pyridinone, A-60253
3-Amino-2(1*H*)-pyridinone, A-60249
3-Amino-4(1*H*)-pyridinone, A-60254
4-Amino-2(1*H*)-pyridinone, A-60250
5-Amino-2(1*H*)-pyridinone, A-60251
6-Amino-2(1*H*)-pyridinone, A-60252
1,1-Cyclopropanedicarboxylic acid; Nitrile, amide, *in* C-80196
6-Methyl-3-pyridazinone, M-70124
4-Methyl-3(2*H*)-pyridazinone, M-70125
5-Methyl-3(2*H*)-pyridazinone, M-70126
6-Methyl-4(1*H*)-pyridazinone, M-80151
1*H*-Pyrazole; *N*-Ac, *in* P-70152

$C_5H_6N_2OS$
5,6-Dihydro-4*H*-cyclopenta-1,2,3-thiadiazole; 2-Oxide, *in* D-70179
3,4-Dihydro-5-methyl-4-thioxo-2(1*H*)-pyrimidinone, D-70233

$C_5H_6N_2O_2$
4-Amino-2(1*H*)-pyridinone; *N*-Oxide, *in* A-60250
1*H*-Imidazole-4-carboxylic acid; Me ester, *in* I-60004

$C_5H_6N_2O_2S$
2-Amino-4-thiazoleacetic acid, A-80146
2-Amino-5-thiazoleacetic acid, A-80147
▷ 2-Thioxo-4-imidazolidinone; 1-*N*-Ac, *in* T-70188

$C_5H_6N_2S$
2-Amino-3-pyridinethiol, A-80136
4-Amino-3-pyridinethiol, A-80137
6-Amino-3-pyridinethiol, A-80138
2-Amino-4(1*H*)-pyridinethione, A-80139
▷ 3-Amino-2(1*H*)-pyridinethione, A-60247
3-Amino-4(1*H*)-pyridinethione, A-80140
5-Amino-2(1*H*)-pyridinethione, A-80141
6-Amino-2(1*H*)-pyridinethione, A-80142
5,6-Dihydro-4*H*-cyclopenta-1,2,3-thiadiazole, D-70179

$C_5H_6N_2S_2$
▷ 5-Methyl-2,4-(1*H*,3*H*)-pyrimidinedithione, M-70127
6-Methyl-2,4(1*H*,3*H*)-pyrimidinedithione, M-70128

$C_5H_6N_2S_3$
6-Mercapto-2,4(1*H*,3*H*)-pyrimidinedithione; 2-*S*-Me, *in* M-80030

$C_5H_6N_4$
2-Amino-3-cyano-4-methylpyrazole, *in* A-80110
4-Amino-3-cyano-5-methylpyrazole, *in* A-80111
5-Amino-4-cyano-1-methylpyrazole, *in* A-70192
3-Amino-1-methyl-4-pyrazolecarbonitrile, *in* A-70187

$C_5H_6N_6O$
8-Aminoguanine, A-80078
2,8-Diamino-1,7-dihydro-6*H*-purin-6-one, D-60035

C_5H_6O
2-Cyclopenten-1-one, C-60226
2-Oxabicyclo[3.1.0]hex-3-ene, O-70056

C_5H_6OS
3-Methoxythiophene, *in* T-60212
▷ 2-Methyl-3-furanthiol, M-70082

$C_5H_6O_2$
Bicyclo[1.1.0]butane-1-carboxylic acid, B-70094
3-Butynoic acid; Me ester, *in* B-70309
4-Hydroxy-2-cyclopentenone, H-60116
▷ 5-Methyl-2(3*H*)-furanone, M-70081
▷ 5-Methyl-2(5*H*)-furanone, M-60083
4-Methyl-3-methylene-2-oxetanone, M-80119
3-Oxabicyclo[3.1.0]hexan-2-one, O-70055
4-Pentene-2,3-dione, P-60061
▷ 4-Pentynoic acid, P-80062

$C_5H_6O_3$
2-Cyclopropyl-2-oxoacetic acid, C-60231
Dimethoxycyclopropenone, *in* D-70290
5-Hydroxymethyl-2(5*H*)-furanone, H-60182
3-Methoxy-2(5*H*)-furanone, M-80043
4-Methoxy-2(5*H*)-furanone, *in* F-80087
3-Methyl-4-oxo-2-butenoic acid, M-70103
3-Oxocyclobutanecarboxylic acid, O-80073
▷ 4-Oxo-2-pentenoic acid, O-70098

$C_5H_6O_4$
1,1-Cyclopropanedicarboxylic acid, C-80196
1,2-Cyclopropanedicarboxylic acid, C-70248
Dihydro-3-methoxy-2,5-furandione, *in* D-80211
Methyl diformylacetate, *in* D-60190

$C_5H_6O_5$
Methyl hydrogen 2-formylmalonate, *in* H-80204
3-Oxopentanedioic acid, O-60084

C_5H_6S
2-Thiabicyclo[3.1.0]hex-3-ene, T-70161

$C_5H_6S_5$
4,5-Dimercapto-1,3-dithiole-2-thione; Di-Me thioether, *in* D-80409

C_5H_7Br
1-Bromo-2,3-dimethylcyclopropene, B-60235
3-Bromo-3-methyl-1-butyne, B-80213
1-Bromo-1,3-pentadiene, B-60311

$C_5H_7BrN_2$
4-Bromo-3,5-dimethylpyrazole, B-70208
3-Bromo-1,5-dimethylpyrazole, *in* B-70252
4-Bromo-1,3-dimethylpyrazole, *in* B-70251
4-Bromo-1,5-dimethylpyrazole, *in* B-70251
5-Bromo-1,3-dimethylpyrazole, *in* B-70252

$C_5H_7BrO_2$
2-Bromomethyl-2-propenoic acid; Me ester, *in* B-70249

C_5H_7Cl
5-Chloro-1,3-pentadiene, C-60121
5-Chloro-1-pentyne, C-70139

C_5H_7ClOS
Tetrahydro-2-thiophenecarboxylic acid; Chloride, *in* T-70099

$C_5H_7ClO_2$
1-Chloro-2,3-pentanedione, C-60123

C_5H_7FO
2-Fluorocyclopentanone, F-60022

$C_5H_7F_3O_2$
3,3,3-Trifluoropropanoic acid; Et ester, *in* T-80284

C_5H_7I
5-Iodo-1-pentyne, I-70054

$C_5H_7IN_2$
3-Iodo-4,5-dimethylpyrazole, I-70032
4-Iodo-3,5-dimethylpyrazole, I-70033
4-Iodo-1,3-dimethylpyrazole, *in* I-70049
4-Iodo-1,5-dimethylpyrazole, *in* I-70049
5-Iodo-1,3-dimethylpyrazole, *in* I-70050

C_5H_7IO
2-Iodocyclopentanone, I-60043
5-Iodo-4-pentenal, I-70052

$C_5H_7IO_2$
1-Iodocyclobutanecarboxylic acid, I-80022
Tetrahydro-3-iodo-2*H*-pyran-2-one, T-60069

C_5H_7NO
4-Cyanobutanal, *in* O-80089
2-Cyclopenten-1-one; Oxime, *in* C-60226
3-Ethoxy-2-propenenitrile, E-80059
2-Hydroxy-3-methyl-2-butenenitrile, H-80198
1-Methyl-1,2-dihydro-3*H*-pyrrol-3-one, *in* D-70262
3-Methyl-2-oxobutanenitrile, *in* M-80129
4-Vinyl-2-azetidinone, V-60008

C_5H_7NOS
2-Acetyl-4,5-dihydrothiazole, A-70041

$C_5H_7NO_2$
4-Aminodihydro-3-methylene-2-(3*H*)furanone, A-70131
3,4-Dihydro-2*H*-pyrrole-2-carboxylic acid, D-80248
3,4-Dihydro-2*H*-pyrrole-5-carboxylic acid, D-80249
3-Methyl-2,5-pyrrolidinedione, M-80155

$C_5H_7NO_2S$
3-(Ethylthio)-2-propenoic acid; Nitrile, *S*-dioxide, *in* E-60055
Tetrahydro-2-thiophenecarboxylic acid; Nitrile, 1,1-dioxide, *in* T-70099

$C_5H_7NO_3$
Methyl 3-amino-2-formyl-2-propenoate, *in* A-80134
2-Nitrocyclopentanone, N-80044
5-Oxo-2-pyrrolidinecarboxylic acid, O-70102

$C_5H_7NO_3S$
5-Oxo-3-thiomorpholinecarboxylic acid, O-80095

$C_5H_7NO_4$
2-Amino-4-hydroxypentanedioic acid; Lactone, *in* A-60195
5-Methyl-2-oxo-4-oxazolidinecarboxylic acid, M-60108
3-Oxopentanedioic acid; Amide, *in* O-60084

$C_5H_7NO_5$
3-Oxopentanedioic acid; Oxime, *in* O-60084

$C_5H_7NO_6$
2-Amino-1,1,2-ethanetricarboxylic acid, A-80072

C_5H_7NS
2-Cyanotetrahydrothiophene, *in* T-70099
3-(Ethylthio)-2-propenoic acid; Nitrile, *in* E-60055

$C_5H_7NS_2$
2-(Ethylthio)thiazole, *in* T-60200

$C_5H_7N_3$
▷ 3-Azido-3-methyl-1-butyne, A-80203

$C_5H_7N_3O$
4-Amino-1,7-dihydro-2*H*-1,3-diazepin-2-one, A-70130
2-Amino-6-methyl-4(1*H*)-pyrimidinone, A-60230
4-Hydrazino-2(1*H*)-pyridinone, H-60093
1*H*-Imidazole-4-carboxylic acid; Methylamide, *in* I-60004

$C_5H_7N_3OS$
2-Amino-5-thiazoleacetic acid; Amide, *in* A-80147

$C_5H_7N_3O_2$
2-Amino-4(5)-imidazoleacetic acid, A-80086
3-Amino-5-methyl-1*H*-pyrazole-4-carboxylic acid, A-80110
4-Amino-5-methyl-1*H*-pyrazole-3-carboxylic acid, A-80111
3-Amino-1*H*-pyrazole-5-carboxylic acid; *N*(1)-Me, *in* A-70188
5-Amino-1*H*-pyrazole-3-carboxylic acid; *N*(1)-Me, *in* A-70191
3-Amino-1*H*-pyrazole-4-carboxylic acid; Me ester, *in* A-70187
3-Azido-2-propenoic acid; Et ester, *in* A-70290
1,6-Dimethyl-5-azauracil, *in* M-60132
3,6-Dimethyl-5-azauracil, *in* M-60132
Methyl 1-methyl-1*H*-1,2,3-triazole-5-carboxylate, *in* T-60239
1*H*-1,2,3-Triazole-4-carboxylic acid; Et ester, *in* T-60239
1*H*-1,2,3-Triazole-4-carboxylic acid; 1-Me, Me ester, *in* T-60239
1*H*-1,2,3-Triazole-4-carboxylic acid; 2-Me, Me ester, *in* T-60239

$C_5H_7N_3O_2S$
2-Pyridinesulfonic acid; Hydrazide, *in* P-70171

$C_5H_7N_3O_3$
Cyanuric acid; 1,3-Di-Me, *in* C-60179

$C_5H_7N_3O_6$
1,1-Dinitro-2-propanone; *O*-Acetyloxime, *in* D-70454

C_5H_8
Methylenecyclobutane, M-70066

$C_5H_8Br_2$
1,1-Dibromo-3-methyl-1-butene, D-60104

$C_5H_8ClNO_2$
1-Chloro-2,3-pentanedione; 2-Oxime, *in* C-60123

$C_5H_8Cl_2$
2,5-Dichloro-1-pentene, D-80126

$C_5H_8Cl_2O$
▷ 3,3-Bis(chloromethyl)oxetane, B-60149
1,5-Dichloro-3-pentanone, D-80125

$C_5H_8FNO_2$
4-Amino-5-fluoro-2-pentenoic acid, A-60161

C_5H_8INO
5-(Iodomethyl)-2-pyrrolidinone, I-80037

$C_5H_8N_2$
1,4-Dihydro-2-methylpyrimidine, D-70225

$C_5H_8N_2O$
3,4-Dihydro-2(1*H*)-pyrimidinone; 1-Me, *in* D-60273
5,6-Dihydro-4(1*H*)-pyrimidinone; 3-Me, *in* D-60274

$C_5H_8N_2OS$
2-Acetyl-4,5-dihydrothiazole: Oxime, *in* A-70041
2-Thioxo-4-imidazolidinone; 1,3-*N*-Di-Me, *in* T-70188

$C_5H_8N_2O_2$
5-Amino-3,4-dihydro-2*H*-pyrrole-2-carboxylic acid, A-70135
3-Amino-2,6-piperidinedione, A-80133
▷ *N*-(2-Cyanoethyl)glycine, *in* C-60016
5-Oxo-2-pyrrolidinecarboxylic acid; Amide, *in* O-70102

$C_5H_8N_2O_5$
N,N'-Carbonylbisglycine, C-80020

$C_5H_8N_2O_7$
3,3-Bis(nitratomethyl)oxetane, *in* O-60056

$C_5H_8N_4$
3-Amino-1,2,4-triazine; *N,N*-Di-Me, *in* A-70203

$C_5H_8N_4O$
6-Amino-2-(methylamino)-4(3*H*)-pyrimidinone, *in* D-70043
4-Amino-5-methyl-1*H*-pyrazole-3-carboxylic acid; Amide, *in* A-80111
5-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Me, amide, *in* A-70192
4-Amino-1,3,5-triazin-2(1*H*)-one; 1,4-*N*-Di-Me, *in* A-80149
4-Amino-1,3,5-triazin-2(1*H*)-one; 4,4-*N*-Di-Me, *in* A-80149
2,6-Diamino-4(1*H*)-pyrimidinone; 1-Me, *in* D-70043

C_5H_8O
2-Methyl-2-butenal, M-80056
▷ 3-Methyl-2-butenal, M-70055
(1-Methylethenyl)oxirane, M-70080
▷ 1-Penten-3-one, P-60062
3-Pentyn-2-ol, P-70041

C_5H_8OS
Tetrahydro-2*H*-pyran-2-thione, T-70085

$C_5H_8OS_2$
3,3-Bis(methylthio)propenal, B-80156

$C_5H_8O_2$
4-Cyclopentene-1,3-diol, C-80193
Dihydro-4-methyl-2(3*H*)-furanone, D-80220
2,6-Dioxaspiro[3.3]heptane, D-60468
2-Ethynyl-1,3-propanediol, E-70054
2-Hydroxycyclopentanone, H-60114
3-Hydroxycyclopentanone, H-60115
2-Hydroxy-2-methylcyclobutanone, H-70168
2-Methyl-3-oxobutanal, M-70102
4-Oxopentanal, O-60083
▷ 2,4-Pentanedione, P-60059
2-Vinyl-1,3-dioxolane, *in* P-70119
3-Vinyl-2-oxiranemethanol, V-80009

$C_5H_8O_2S$
2,3-Dihydro-2-methylthiophene; 1,1-Dioxide, *in* D-70227
2,3-Dihydro-5-methylthiophene; 1,1-Dioxide, *in* D-70229
3-(Ethylthio)-2-propenoic acid, E-60055
Isoprene cyclic sulfone, *in* D-70231
α-Isoprene sulfone, *in* D-70228
4-Mercapto-2-butenoic acid; Me ester, *in* M-60018
2-Methyl-3-sulfolene, *in* D-70230
Tetrahydro-2-thiophenecarboxylic acid, T-70099

$C_5H_8O_2Se$
3-Selenetanol; Ac, *in* S-80022

$C_5H_8O_3$
Dihydro-4-hydroxy-3-methyl-2(3*H*)-furanone, D-80214
Dihydro-4-hydroxy-5-methyl-2(3*H*)furanone, *in* D-80353
2-Ethoxy-2-propenoic acid, E-70037
3-Methyloxiranecarboxylic acid; Me ester, *in* M-80127
3-Methyl-2-oxobutanoic acid, M-80129
4-Oxobutanoic acid; Me ester, *in* O-80068
5-Oxopentanoic acid, O-80089

$C_5H_8O_3S$
2-Mercaptopropanoic acid; *S*-Ac, *in* M-60027

$C_5H_8O_4$
4,5-Dihydro-3-hydroxy-5-(hydroxymethyl)-2(3*H*)-furanone, D-70212
Methylpropanedioic acid; Mono-Me ester, *in* M-80149

C_5H_8S
2,3-Dihydro-2-methylthiophene, D-70227
2,3-Dihydro-4-methylthiophene, D-70228
2,3-Dihydro-5-methylthiophene, D-70229
2,5-Dihydro-2-methylthiophene, D-70230
2,5-Dihydro-3-methylthiophene, D-70231

$C_5H_8S_2$
2-Vinyl-1,3-dithiolane, *in* P-70119

C_5H_9BrO
5-Bromopentanal, B-70263
2-Bromotetrahydro-2*H*-pyran, B-70271

$C_5H_9BrO_2$
2-Bromo-2-methylpropanoic acid; Me ester, *in* B-80229

$C_5H_9ClN_4$
5-Chlorotetrazole; 1-*tert*-Butyl, *in* C-80113
5-Chlorotetrazole; 2-*tert*-Butyl, *in* C-80113

C_5H_9ClO
5-Chloropentanal, C-70137
4-Chloro-4-penten-1-ol, C-80091
2-Chlorotetrahydro-2*H*-pyran, C-80110
3-Chlorotetrahydro-2*H*-pyran, C-80111
4-Chlorotetrahydro-2*H*-pyran, C-80112

C_5H_9ClOS
Carbonochloridothioic acid; *O*-Butyl, *in* C-60013
Carbonochloridothioic acid; *O*-*tert*-Butyl, *in* C-60013
Carbonochloridothioic acid; *S*-Butyl, *in* C-60013

$C_5H_9ClO_2$
3-Chloro-2-(methoxymethoxy)-1-propene, C-70089

$C_5H_9ClO_3$
(1-Chloroethyl) ethyl carbonate, C-60067
2-(Chloromethoxy)ethyl acetate, C-70088

$C_5H_9FN_2$
2-Amino-3-fluoro-3-methylbutanoic acid; Nitrile, *in* A-60159

$C_5H_9IN_2$
1,3-Dimethyl-1*H*-imidazolium(1+); Iodide, *in* D-80451

C_5H_9IO
2-Iodo-3-methylbutanal, I-60049
2-Iodopentanal, I-60054
5-Iodo-2-pentanone, I-60057
5-Iodo-4-penten-1-ol, I-60058

C_5H_9N
3,4-Dihydro-5-methyl-2*H*-pyrrole, D-70226
▷ 1-Isocyanobutane, I-80058
4-Pentyn-1-amine, P-80061
2-Propyn-1-amine; *N*-Di-Me, *in* P-60184
▷ 1,2,3,6-Tetrahydropyridine, T-70089
2,3,4,5-Tetrahydropyridine, T-70090

C_5H_9NO
4,5-Dihydro-4,4-dimethyloxazole, D-70198
3,4-Dihydro-5-methoxy-2*H*-pyrrole, *in* P-70188
4-Imino-2-pentanone, *in* P-60059
2-Pyrrolidinecarboxaldehyde, P-70184
Tiglic aldehyde; Oxime, *in* M-80056

$C_5H_9NO_2$
2-Amino-3-methyl-3-butenoic acid, A-60218
5-(Aminomethyl)dihydro-2(3*H*)-furanone, *in* A-60196
3,5-Dimethyl-2-oxazolidinone, *in* M-60107
2-Ethoxy-2-propenoic acid; Amide, *in* E-70037
2-Hydroxycyclopentanone; Oxime, *in* H-60114
3-Methyl-2-oxobutanoic acid; Amide, *in* M-80129

$C_5H_9NO_2S$
3-Aminotetrahydro-3-thiophenecarboxylic acid, A-70199
2-Thiazolidineacetic acid, T-80173
3-Thiomorpholinecarboxylic acid, T-70182

$C_5H_9NO_3$
2-Amino-2-(hydroxymethyl)-3-butenoic acid, A-60187
1-Amino-2-(hydroxymethyl)cyclopropanecarboxylic acid, A-80083
3,4-Dihydro-3,4-dihydroxy-2-(hydroxymethyl)-2*H*-pyrrole, D-60222
3-Methyl-2-oxobutanoic acid; Oxime, *in* M-80129
3-Morpholinecarboxylic acid, M-70155

$C_5H_9NO_4$
2-Amino-3-methylbutanedioic acid, A-70166
3-(Carboxymethylamino)propanoic acid, C-60016
3,4-Dihydroxy-2-pyrrolidinecarboxylic acid, D-70342
3-Nitro-1-propanol; Ac, *in* N-60039
Threonine; *N*-Formyl, *in* T-60217

$C_5H_9NO_5$
2-Amino-4-hydroxypentanedioic acid, A-60195

C_5H_9NS
2,3-Dihydro-2,2-dimethylthiazole, D-80194
▷ 2-Isothiocyanato-2-methylpropane, I-70105
2-Methyl-2-thiocyanatopropane, M-70135
2-Propenethioamide; *N,N*-Di-Me, *in* P-70120
2-Pyrrolidinethione; *N*-Me, *in* P-70186

$C_5H_9NS_2$
5,6-Dihydro-2-(methylthio)-4*H*-1,3-thiazine, *in* T-60094
Tetrahydro-2*H*-1,3-thiazine-2-thione; *N*-Me, *in* T-60094

$C_5H_9N_2^{\oplus}$
1,3-Dimethyl-1*H*-imidazolium(1+), D-80451

$C_5H_9N_2S_2$
5-*tert*-Butyl-1,2,3,5-dithiadiazolyl, B-70302
5-*tert*-Butyl-1,3,2,4-dithiadiazolyl, B-70303

$C_5H_9N_3O$
3,5-Dihydro-3,5,5-trimethyl-4*H*-triazol-4-one, D-60303

$C_5H_9N_3O_2$
3-Azido-3-methylbutanoic acid, A-60348

$C_5H_9N_4O$
Porphyrexide, P-70110

$C_5H_9N_5$
2,4,6-Triaminopyrimidine; N^4-Me, *in* T-80208

$C_5H_9N_5O$
4-Amino-5-methyl-1*H*-pyrazole-3-carboxylic acid; Hydrazide, *in* A-80111
2,4,6-Triaminopyrimidine; N^4-Me, N^1-oxide, *in* T-80208

$C_5H_{10}ClN$
1-Methylenepyrrolidinium(1+); Chloride, *in* M-70077

$C_5H_{10}ClNO_2$
2-Amino-3-chlorobutanoic acid; Me ester, *in* A-60103
2-Amino-4-chlorobutanoic acid; Me ester, *in* A-60104

$C_5H_{10}Cl_2O$
1,5-Dichloro-3-pentanol, D-80124

$C_5H_{10}FNO_2$
2-Amino-3-fluoro-3-methylbutanoic acid, A-60159
2-Amino-3-fluoropentanoic acid, A-60160

$C_5H_{10}N^{\oplus}$
1-Methylenepyrrolidinium(1+), M-70077

$C_5H_{10}N_2$
2-Amino-2-methylbutanoic acid; Nitrile, *in* A-70167
2,5-Diazabicyclo[4.1.0]heptane, D-60053

$C_5H_{10}N_2O$
▷ 1,3-Dimethylimidazolidinone, *in* I-70005
Tetrahydro-2(1*H*)-pyrimidinone; 1-Me, *in* T-60088
Tetrahydro-4(1*H*)-pyrimidinone; 3-Me, *in* T-60089

$C_5H_{10}N_2O_2$
4-Oxopentanal; Dioxime, *in* O-60083
2,4-Pentanedione; Dioxime, *in* P-60059

$C_5H_{10}N_2O_4$
▷ 2,4-Dinitropentane, D-70453

$C_5H_{10}N_2O_5$
4,5-Dihydroxy-1,3-bis(hydroxymethyl)-2-imidazolidinone, D-80301

$C_5H_{10}O$
2,3-Dimethylcyclopropanol, D-70397
2-Methyl-2-buten-1-ol, M-80057

$C_5H_{10}OSe$
Methaneselenoic acid; *tert*-Butyl ester, *in* M-70035

$C_5H_{10}O_2$
1,2-Cyclopentanediol, C-80189
▷ 3,3-Dimethoxypropene, *in* P-70119
3,3-Dimethyl-1,2-dioxolane, D-80446
2,3-Dimethyloxiranemethanol, D-80462
3,3-Dimethyloxiranemethanol, D-70426
2-Methoxybutanal, *in* H-70112
1-Methoxy-3-buten-2-ol, *in* B-70291

$C_5H_{10}O_2S$
2-Mercapto-3-methylbutanoic acid, M-60023
2-Mercaptopropanoic acid; Et ester, *in* M-60027
2-Mercaptopropanoic acid; Me ester, *S*-Me ether, *in* M-60027

$C_5H_{10}O_2S_2$
1,2-Dithiepane; 1,1-Dioxide, *in* D-70517

$C_5H_{10}O_3$
3,3-Oxetanedimethanol, O-60056

$C_5H_{10}O_4$
2,3-Dihydroxybutanoic acid; Me ester, *in* D-60312
3,4-Dihydroxypentanoic acid, D-80353
▷ Glycerol 1-acetate, G-60029

$C_5H_{10}O_4S_2$
1,2-Dithiepane; 1,1,2,2-Tetraoxide, *in* D-70517

$C_5H_{10}S_2$
1,1-Cyclopentanedithiol, C-60222
1,1-Cyclopropanedimethanethiol, C-70249
1,2-Dithiepane, D-70517
5-Methyl-1,3-dithiane, M-60067

$C_5H_{10}S_3$
Carbonotrithioic acid; Di-Et ester, *in* C-80019

$C_5H_{11}BrO$
3-Bromo-2,2-dimethylpropanol, B-80200
5-Bromo-2-pentanol, B-60313

$C_5H_{11}ClO$
tert-Butyl chloromethyl ether, B-70295
1-Chloro-3-pentanol, C-70138

$C_5H_{11}ClO_2S$
(2-Carboxyethyl)dimethylsulfonium(1+); Chloride, *in* C-80024

$C_5H_{11}IO$
1-Iodo-3-pentanol, I-60055
5-Iodo-2-pentanol, I-60056

$C_5H_{11}NOS$
3-Aminotetrahydro-2*H*-thiopyran; *S*-Oxide, *in* A-70200

$C_5H_{11}NO_2$
2-Amino-2-methylbutanoic acid, A-70167
3-Amino-2-methylbutanoic acid, A-80097

$C_5H_{11}NO_2S$
3-Aminotetrahydro-2*H*-thiopyran; *S,S*-Dioxide, *in* A-70200

$C_5H_{11}NO_3$
2-Amino-4-hydroxy-2-methylbutanoic acid, A-60186
4-Amino-5-hydroxypentanoic acid, A-70159
5-Amino-4-hydroxypentanoic acid, A-60196
3-Amino-2-hydroxypropanoic acid; Et ester, *in* A-70160
Threonine; *N*-Me, *in* T-60217
Threonine; Me ester, *in* T-60217
Threonine; Me ether, *in* T-60217

$C_5H_{11}NO_4$
1,1-Dimethoxy-3-nitropropane, *in* N-60037

$C_5H_{11}NS$
3-Aminotetrahydro-2*H*-thiopyran, A-70200
2-Pyrrolidinemethanethiol, P-70185

$C_5H_{11}N_3$
1-Azido-2,2-dimethylpropane, A-60344

$C_5H_{11}N_3O_2$
Biuret; 1,3,5-Tri-Me, *in* B-60190

$C_5H_{11}O_2S^{\oplus}$
(2-Carboxyethyl)dimethylsulfonium(1+), C-80024

$C_5H_{12}N_2O$
3,3-Bis(aminomethyl)oxetane, B-60140

$C_5H_{12}N_2O_2S$
S-(2-Aminoethyl)cysteine, A-60152

$C_5H_{12}N_2O_3$
2,5-Diamino-3-hydroxypentanoic acid, D-70039

$C_5H_{12}N_2O_3S$
S-(2-Aminoethyl)cysteine; *S*-Oxide, *in* A-60152
Aminoiminomethanesulfonic acid; *N*-*tert*-Butyl, *in* A-60210
Methionine sulfoximine, M-70043

$C_5H_{12}N_2O_4S$
S-(2-Aminoethyl)cysteine; *S,S*-Dioxide, *in* A-60152

$C_5H_{12}N_2S$
▷ *N,N'*-Diethylthiourea, D-70155

$C_5H_{12}N_2Se$
Selenourea; *N*-Tetra-Me, *in* S-70031

$C_5H_{12}O_2$
2-Methyl-1,3-butanediol, M-80054
3-Methyl-1,2-butanediol, M-80055
2,3-Pentanediol, P-80060

$C_5H_{12}O_2S$
1,1-Dimethoxy-2(methylthio)ethane, *in* M-80017

$C_5H_{12}O_3$
2-(Hydroxymethyl)-1,4-butanediol, H-80197

$C_5H_{12}O_4S_4$
Tris(methylthio)methylium(1+); Methylsulfate, *in* T-80367

$C_5H_{12}O_4S_5$
Dysoxysulfone, D-80539

$C_5H_{12}S_2$
2,2-Dimethyl-1,3-propanedithiol, D-70433

$C_5H_{12}S_3$
2-Mercaptomethyl-2-methyl-1,3-propanedithiol, M-70030

$C_5H_{12}S_4$
2,2-Bis(mercaptomethyl)-1,3-propanedithiol, B-60164

$C_5H_{13}NO$
3-Amino-3-methyl-2-butanol, A-60217

$C_5H_{13}NO_2$
1-Amino-3-methyl-2,3-butanediol, A-60216
2-Amino-1,5-pentanediol, A-80131

$C_5H_{14}N_2$
2,4-Pentanediamine, P-70039

C_5O_2
1,2,3,4-Pentatetraene-1,5-dione, P-70040

$C_6BrF_4NO_2$
1-Bromo-2,3,4,5-tetrafluoro-6-nitrobenzene, B-60323

1-Bromo-2,3,4,6-tetrafluoro-5-nitrobenzene, B-60324
1-Bromo-2,3,5,6-tetrafluoro-4-nitrobenzene, B-60325

C_6BrF_{13}
1-Bromo-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexane, B-70274

$C_6Br_2F_4$
1,2-Dibromo-3,4,5,6-tetrafluorobenzene, D-60106
1,3-Dibromo-2,4,5,6-tetrafluorobenzene, D-60107
1,4-Dibromo-2,3,5,6-tetrafluorobenzene, D-60108

$C_6Br_3F_3$
1,3,5-Tribromo-2,4,6-trifluorobenzene, T-70214

C_6ClF_{13}
1-Chloro-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexane, C-70163

$C_6Cl_2F_4$
1,2-Dichloro-3,4,5,6-tetrafluorobenzene, D-60151
1,3-Dichloro-2,4,5,6-tetrafluorobenzene, D-60152
1,4-Dichloro-2,3,5,6-tetrafluorobenzene, D-60153

$C_6Cl_2N_4$
2,3-Dichloro-5,6-dicyanopyrazine, *in* D-80129

$C_6Cl_3F_3$
1,2,3-Trichloro-4,5,6-trifluorobenzene, T-60256
▷ 1,3,5-Trichloro-2,4,6-trifluorobenzene, T-60257

$C_6F_4I_2$
1,2,3,4-Tetrafluoro-5,6-diiodobenzene, T-60044
1,2,3,5-Tetrafluoro-4,6-diiodobenzene, T-60045
▷ 1,2,4,5-Tetrafluoro-3,6-diiodobenzene, T-60046

C_6F_5IO
Pentafluoroiodosobenzene, P-60034

C_6F_5NO
Pentafluoronitrosobenzene, P-60039

$C_6F_5NO_2$
Pentafluoronitrobenzene, P-80026

$C_6F_5N_3$
Azidopentafluorobenzene, A-60350

$C_6F_{12}OS_2$
2,2,4,4-Tetrakis(trifluoromethyl)-1,3-dithietane; 1-Oxide, *in* T-60129

$C_6F_{12}O_2S_2$
2,2,4,4-Tetrakis(trifluoromethyl)-1,3-dithietane; 1,1-Dioxide, *in* T-60129
2,2,4,4-Tetrakis(trifluoromethyl)-1,3-dithietane; 1,3-Dioxide, *in* T-60129

$C_6F_{12}O_3S_2$
2,2,4,4-Tetrakis(trifluoromethyl)-1,3-dithietane; 1,1,3-Trioxide, *in* T-60129

$C_6F_{12}O_4S_2$
2,2,4,4-Tetrakis(trifluoromethyl)-1,3-dithietane; 1,1,3,3-Tetraoxide, *in* T-60129

$C_6F_{12}S_2$
▷ 2,2,4,4-Tetrakis(trifluoromethyl)-1,3-dithietane, T-60129

$C_6F_{12}S_4$
Tetrakis(trifluoromethylthio)ethene, T-80132

C_6HBrF_4
1-Bromo-2,3,4,5-tetrafluorobenzene, B-60320
2-Bromo-1,3,4,5-tetrafluorobenzene, B-60321
3-Bromo-1,2,4,5-tetrafluorobenzene, B-60322

$C_6HClN_4O_8$
▷ 3-Chloro-1,2,4,5-tetranitrobenzene, C-60135

$C_6HCl_4N_3$
4,5,6,7-Tetrachlorobenzotriazole, T-60027

$C_6HF_4N_3$
4,5,6,7-Tetrafluoro-1*H*-benzotriazole, T-70035

$C_6H_2BrFN_2O_4$
1-Bromo-2-fluoro-3,5-dinitrobenzene, B-60246

$C_6H_2Br_2F_2$
1,2-Dibromo-4,5-difluorobenzene, D-80087
1,4-Dibromo-2,5-difluorobenzene, D-80088

$C_6H_2Br_2I_2O_2$
4,5-Dibromo-3,6-diiodo-1,2-benzenediol, D-80090

$C_6H_2Br_2O_2$
2,6-Dibromo-1,4-benzoquinone, D-60088

$C_6H_2ClN_5O_8$
▷ 2-Chloro-3,4,5,6-tetranitroaniline, C-60134

$C_6H_2Cl_2N_2O_4$
5,6-Dichloro-2,3-pyrazinedicarboxylic acid, D-80129

$C_6H_2Cl_3I$
1,2,3-Trichloro-4-iodobenzene, T-80227

$C_6H_2F_3NO_2$
1,2,3-Trifluoro-4-nitrobenzene, T-60299
1,2,3-Trifluoro-5-nitrobenzene, T-60300
▷ 1,2,4-Trifluoro-5-nitrobenzene, T-60301
1,2,5-Trifluoro-3-nitrobenzene, T-60302
1,2,5-Trifluoro-4-nitrobenzene, T-60303
1,3,5-Trifluoro-2-nitrobenzene, T-60304

$C_6H_2I_2N_2O_4$
1,2-Diiodo-3,5-dinitrobenzene, D-80398
1,2-Diiodo-4,5-dinitrobenzene, D-80399
1,3-Diiodo-4,6-dinitrobenzene, D-80400

$C_6H_2O_6$
5,6-Dihydroxy-5-cyclohexene-1,2,3,4-tetrone, D-60315

$C_6H_3BrCl_2O$
2-Bromo-3,5-dichlorophenol, B-60226
2-Bromo-4,5-dichlorophenol, B-60227
3-Bromo-2,4-dichlorophenol, B-60228
4-Bromo-2,3-dichlorophenol, B-60229
4-Bromo-3,5-dichlorophenol, B-60230

$C_6H_3BrINO_2$
1-Bromo-2-iodo-3-nitrobenzene, B-70222
2-Bromo-1-iodo-3-nitrobenzene, B-70223

$C_6H_3Br_2NO_2$
2,6-Dibromo-4-nitroso-1-naphthol, *in* D-60088

$C_6H_3Cl_2NO_3$
2,3-Dichloro-4-nitrophenol, D-70125

$C_6H_3Cl_4NO_2S$
2,3,4,5-Tetrachloro-1,1-dihydro-1-[(methoxycarbonyl)imino]thiophene, T-60028

$C_6H_3FN_4O_2$
▷ 4-Azido-1-fluoro-2-nitrobenzene, A-80199

$C_6H_3N_3O_3$
▷ 4-Diazo-2-nitrophenol, D-60065
1,3,5-Triazine-2,4,6-tricarboxaldehyde, T-60237

$C_6H_3N_3O_9S$
▷ 2,4,6-Trinitrobenzenesulfonic acid, T-70302

$C_6H_3N_5O_8$
▷ 2,3,4,6-Tetranitroaniline, T-60159

C_6H_4
Benzyne, B-70087

C_6H_4BrFO
2-Bromo-3-fluorophenol, B-60247
2-Bromo-4-fluorophenol, B-60248
2-Bromo-6-fluorophenol, B-60249
3-Bromo-4-fluorophenol, B-60250
4-Bromo-2-fluorophenol, B-60251

$C_6H_4BrNO_3$
2-Bromo-3-nitrophenol, B-70257

$C_6H_4BrNS_2$
1,3,2-Benzodithiazol-1-ium(1+); Bromide, *in* B-70033

$C_6H_4BrN_3$
3-Bromo[1,2,3]triazolo[1,5-*a*]pyridine, B-60329
7-Bromo[1,2,3]triazolo[1,5-*a*]pyridine, B-60330

$C_6H_4Br_4N_2$
2,3-Bis(dibromomethyl)pyrazine, B-60150
4,5-Bis(dibromomethyl)pyrimidine, B-60153

C_6H_4ClFO
2-Chloro-4-fluorophenol, C-60073
2-Chloro-5-fluorophenol, C-60074
2-Chloro-6-fluorophenol, C-60075
3-Chloro-2-fluorophenol, C-60076
▷ 3-Chloro-4-fluorophenol, C-60077
3-Chloro-5-fluorophenol, C-60078
4-Chloro-2-fluorophenol, C-60079
4-Chloro-3-fluorophenol, C-60080

C_6H_4ClFS
3-Chloro-4-fluorobenzenethiol, C-60069
4-Chloro-2-fluorobenzenethiol, C-60070
4-Chloro-3-fluorobenzenethiol, C-60071

C_6H_4ClNO
1-Chloro-2-nitrosobenzene, C-80083
1-Chloro-3-nitrosobenzene, C-80084
1-Chloro-4-nitrosobenzene, C-80085

$C_6H_4ClNO_3$
▷ 5-Chloro-2-nitrophenol, C-60119

$C_6H_4ClNS_2$
1,3,2-Benzodithiazol-1-ium(1+); Chloride, *in* B-70033

$C_6H_4ClN_3$
4-Chloro-1*H*-imidazo[4,5-*c*]pyridine, C-60104
6-Chloro-1*H*-imidazo[4,5-*c*]pyridine, C-60105

$C_6H_4Cl_2S$
2,3-Dichlorobenzenethiol, D-60119
2,4-Dichlorobenzenethiol, D-60120
2,5-Dichlorobenzenethiol, D-60121
2,6-Dichlorobenzenethiol, D-60122
3,4-Dichlorobenzenethiol, D-60123
3,5-Dichlorobenzenethiol, D-60124

$C_6H_4Cl_3NO$
2-(Trichloroacetyl)pyrrole, T-80221

C_6H_4FNO
5-Fluoro-3-pyridinecarboxaldehyde, F-80060

$C_6H_4FNO_3$
▷ 5-Fluoro-2-nitrophenol, F-60061

$C_6H_4FN_3O_4$
2-Fluoro-3,5-dinitroaniline, F-60027
2-Fluoro-4,6-dinitroaniline, F-60028
4-Fluoro-2,6-dinitroaniline, F-60029
4-Fluoro-3,5-dinitroaniline, F-60030
5-Fluoro-2,4-dinitroaniline, F-60031
6-Fluoro-3,4-dinitroaniline, F-60032

$C_6H_4F_2N_2O_2$
5-(2,2-Difluorovinyl)uracil, D-80167

$C_6H_4F_2S$
2,5-Difluorobenzenethiol, D-60173
2,6-Difluorobenzenethiol, D-60174
3,4-Difluorobenzenethiol, D-60175
3,5-Difluorobenzenethiol, D-60176

$C_6H_4F_3N$
2-(Trifluoromethyl)pyridine, T-60296
3-(Trifluoromethyl)pyridine, T-60297
4-(Trifluoromethyl)pyridine, T-60298

$C_6H_4F_3NO$
2-(Trifluoromethyl)pyridine; 1-Oxide, *in* T-60296
3-(Trifluoromethyl)pyridine; 1-Oxide, *in* T-60297
4-(Trifluoromethyl)pyridine; 1-Oxide, *in* T-60298

$C_6H_4F_3NO_3S$
2-Pyridinyl trifluoromethanesulfonate, P-70173

$C_6H_4NS_2^{\oplus}$
1,3,2-Benzodithiazol-1-ium(1+), B-70033

$C_6H_4N_2$
Bis(methylene)butanedinitrile, *in* D-70409

$C_6H_4N_2O$
6-Diazo-2,4-cyclohexadien-1-one, D-70057
Furo[2,3-*d*]pyridazine, F-60091
Furo[3,4-*d*]pyridazine, F-60092
3-Isocyanatopyridine, I-70065
5*H*-Pyrrolo[1,2-*a*]imidazol-5-one, P-70194
5*H*-Pyrrolo[1,2-*c*]imidazol-5-one, P-70195
6*H*-Pyrrolo[1,2-*b*]pyrazol-6-one, P-70199

$C_6H_4N_2OS$
▷ 2*H*-[1,2,4]Oxadiazolo[2,3-*a*]pyridine-2-thione, O-70062

$C_6H_4N_2O_2$
5-Ethynyl-2,4(1*H*,3*H*)-pyrimidinedione, E-60060
Furo[2,3-*d*]pyrimidin-2(1*H*)-one, F-60106
4-Hydroxyfuro[2,3-*d*]pyridazine, H-60146
7-Hydroxyfuro[2,3-*d*]pyridazine, H-60147
1,3,4-Oxadiazolo[3,2-*a*]pyridin-2(3*H*)-one, O-70063
2*H*-[1,2,4]Oxadiazolo[2,3-*a*]pyridin-2-one, O-70064
3-Oxopyrazolo[1,2-*a*]pyrazol-8-ylium-1-olate, O-60092

$C_6H_4N_2O_4$
3,6-Pyridazinedicarboxylic acid, P-70168

$C_6H_4N_2O_6$
4,5-Dinitro-1,2-benzenediol, D-70449
▷ 4,6-Dinitro-1,3-benzenediol, D-80491

$C_6H_4N_2S$
2-Isothiocyanatopyridine, I-70106
3-Isothiocyanatopyridine, I-70107
Thiazolo[4,5-*b*]pyridine, T-70166
Thiazolo[5,4-*b*]pyridine, T-70168
Thiazolo[4,5-*c*]pyridine, T-70167
Thiazolo[5,4-*c*]pyridine, T-70169
Thieno[3,2-*d*]pyrimidine, T-60205

$C_6H_4N_2S_2$
2,2′-Bithiazole, B-70166
2,4′-Bithiazole, B-70167
2,5′-Bithiazole, B-70168
4,4′-Bithiazole, B-70169
4,5′-Bithiazole, B-70170
5,5′-Bithiazole, B-70171

$C_6H_4N_2S_4$
2,2′-Dithiobisthiazole, *in* T-60200

$C_6H_4N_4O$
Pyrido[3,4-*d*]-1,2,3-triazin-4(3*H*)-one, P-60238

$C_6H_4N_4O_2$
2,4(1*H*,3*H*)-Pteridinedione, P-60191

$C_6H_4N_4O_3$
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione, P-70134
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione, P-70135

$C_6H_4N_4O_6$
▷ 2,4,6-Trinitroaniline, T-70301

$C_6H_4N_6$
4-Azido-1*H*-imidazo[4,5-*c*]pyridine, A-60345
1*H*-1,2,4-Triazolo[3,4-*i*]purine, T-80212
1*H*-1,2,4-Triazolo[5,1-*i*]purine, T-80213

C_6H_4O
1,5-Hexadiyn-3-one, H-60040
3,5-Hexadiyn-2-one, H-60041

C_6H_4OS
Thieno[3,4-*b*]furan, T-60204

$C_6H_4O_2$
▷ 1,4-Benzoquinone, B-70044
Tricyclo[3.1.0.0^{2,6}]hexanedione, T-70229

$C_6H_4O_4$
3,6-Dihydroxy-1,2-benzoquinone, D-60309

$C_6H_4O_5$
Aconitic acid; Anhydride, *in* A-70055

$C_6H_4O_6$
3,5-Dihydroxy-4-oxo-4*H*-pyran-2-carboxylic acid, D-60368

$C_6H_4O_8$
Ethylenetetracarboxylic acid, E-60049

C_6H_4S
2-Ethynylthiophene, E-70055

C_6H_4SSe
Selenolo[3,4-*b*]thiophene, S-70030

$C_6H_4S_4$
Bi(1,3-dithiol-2-ylidene), B-70119
[1,4]Dithiino[2,3-*b*]-1,4-dithiin, D-70521

$C_6H_4S_6$
Thieno[3,4-*c*]thiophene-1,3,4,6-tetrathiol, T-70170

$C_6H_4S_8$
Tetramercaptotetrathiafulvalene, T-70130

$C_6H_4Se_4$
Bi(1,3-diselenol-2-ylidene), B-70116

$C_6H_4Te_4$
Bi(1,3-ditellurol-2-ylidene), B-70117

C_6H_5BrClN
2-(Bromomethyl)-6-chloropyridine, B-70235
3-(Bromomethyl)-2-chloropyridine, B-70236
4-(Bromomethyl)-2-chloropyridine, B-70237
5-(Bromomethyl)-2-chloropyridine, B-70238

$C_6H_5BrClNO$
4-(Bromomethyl)-2-chloropyridine; 1-Oxide, *in* B-70237

C_6H_5BrFN
2-(Bromomethyl)-6-fluoropyridine, B-70243
3-(Bromomethyl)-2-fluoropyridine, B-70244
4-(Bromomethyl)-2-fluoropyridine, B-70245
5-(Bromomethyl)-2-fluoropyridine, B-70246

C_6H_5BrIN
5-Bromo-2-iodoaniline, B-60279

$C_6H_5BrO_3$
2-Bromo-1,3,5-benzenetriol, B-60199
3-Bromo-1,2,4-benzenetriol, B-70180
4-Bromo-1,2,3-benzenetriol, B-60200
5-Bromo-1,2,3-benzenetriol, B-60201
5-Bromo-1,2,4-benzenetriol, B-70181
6-Bromo-1,2,4-benzenetriol, B-70182
2-Bromo-5,6-epoxy-4-hydroxy-2-cyclohexen-1-one, B-60239

$C_6H_5Br_2NO$
2,4-Dibromo-6-methoxypyridine, *in* D-80100
2,6-Dibromo-4-methoxypyridine, *in* D-80099

$C_6H_5Br_3Se$
Tribromophenylselenium, T-70213

$C_6H_5Cl_2N$
2,3-Dichloro-5-methylpyridine, D-60138
2,5-Dichloro-3-methylpyridine, D-60139

$C_6H_5Cl_2NO$
4-Amino-2,5-dichlorophenol, A-70129

$C_6H_5Cl_3O_2$
2,3-Dihydro-4-(trichloroacetyl)furan, D-70271

$C_6H_5Cl_3Se$
Trichlorophenylselenium, T-70224

$C_6H_5FO_2$
4-Fluoro-1,2-benzenediol, F-60020
4-Fluoro-1,3-benzenediol, F-70018

C_6H_5FS
2-Fluorobenzenethiol, F-80018
3-Fluorobenzenethiol, F-80019
4-Fluorobenzenethiol, F-80020

$C_6H_5F_3O_2$
2,3-Dihydro-4-(trifluoroacetyl)furan, D-70274
2-Trifluoromethyl-1,3-cyclopentanedione, T-80281

$C_6H_5F_4NO_3S$
1-Fluoropyridinium; Trifluoromethanesulfonate, *in* F-60066

$C_6H_5NO_2$
Amino-1,4-benzoquinone, A-60089

$C_6H_5NO_3$
2-Formyl-1*H*-pyrrole-3-carboxylic acid, F-80077
4-Formyl-1*H*-pyrrole-2-carboxylic acid, F-80078
5-Formyl-1*H*-pyrrole-2-carboxylic acid, F-80079
α-Oxo-1*H*-pyrrole-3-acetic acid, O-70101

$C_6H_5NO_4$
1*H*-Pyrrole-3,4-dicarboxylic acid, P-70183

$C_6H_5NO_4S$
4-Nitro-2-thiophenecarboxylic acid; Me ester, *in* N-80061
5-Nitro-2-thiophenecarboxylic acid; Me ester, *in* N-80062

$C_6H_5NO_5$
3-Hydroxy-1*H*-pyrrole-2,4-dicarboxylic acid, H-80251
3-Hydroxy-1*H*-pyrrole-2,5-dicarboxylic acid, H-80252

C_6H_5NS
5*H*-Thieno[2,3-*c*]pyrrole, T-60206

$C_6H_5N_2OS$
3,4-Dihydro-6-methyl-4-thioxo-2(1*H*)-pyrimidinone, D-70234

$C_6H_5N_3$
▷ 1*H*-Benzotriazole, B-70068
Imidazo[1,2-*a*]pyrazine, I-60005
Imidazo[1,2-*b*]pyridazine, I-60007
▷ Imidazo[4,5-*c*]pyridine, I-60008
1*H*-Pyrazolo[3,4-*b*]pyridine, P-70155
5*H*-Pyrrolo[2,3-*b*]pyrazine, P-60248

$C_6H_5N_3O$
4-Amino-5-ethynyl-2(1*H*)-pyrimidinone, A-60153
1,3-Dihydro-2*H*-imidazo[4,5-*b*]pyridin-2-one, D-60249
1,3-Dihydro-2*H*-imidazo[4,5-*c*]pyridin-2-one, D-60250
4-Hydroxyimidazo[4,5-*b*]pyridine, H-60157

$C_6H_5N_5O$
2-Amino-4(1*H*)-pteridinone, A-60242

$C_6H_5N_5O_2$
2-Amino-4(1*H*)-pteridinone; 8-Oxide, *in* A-60242
▷ Isoxanthopterin, I-60141

C_6H_6
2-Ethynyl-1,3-butadiene, E-80073
1,2-Hexadien-5-yne, H-70040
1,3-Hexadien-5-yne, H-70041

C_6H_6BrN
2-(Bromomethyl)pyridine, B-70253
3-(Bromomethyl)pyridine, B-70254
4-(Bromomethyl)pyridine, B-70255

C_6H_6BrNO
3-Amino-2-bromophenol, A-70099
2-Bromo-3-hydroxy-6-methylpyridine, B-60267
2-Bromo-3-methoxypyridine, *in* B-60275
3-Bromo-5-methoxypyridine, *in* B-60277

$C_6H_6BrNO_2$
2-Bromo-3-hydroxy-6-methylpyridine; *N*-Oxide, *in* B-60267
2-Bromo-3-hydroxypyridine; Me ether, *N*-Oxide, *in* B-60275

$C_6H_6BrNO_2S$
2-Bromo-6-(methylsulfonyl)pyridine, *in* B-80256
5-Bromo-2-(methylsulfonyl)pyridine, *in* B-60317

C_6H_6BrNS
2-Bromo-6-(methylthio)pyridine, *in* B-80256
3-Bromo-2-(methylthio)pyridine, *in* B-60315
5-Bromo-2-(methylthio)pyridine, *in* B-60317

$C_6H_6Br_2N_2O_2$
4,5-Dibromo-1*H*-imidazole-2-carboxylic acid; Et ester, *in* D-60102

$C_6H_6Br_2O_3$
2,6-Dibromo-4,5-dihydroxy-2-cyclohexen-1-one, D-60097

$C_6H_6Br_2S$
2,3-Bis(bromomethyl)thiopene, B-80137
2,5-Bis(bromomethyl)thiophene, B-80138
3,4-Bis(bromomethyl)thiophene, B-80139

C_6H_6ClNO
2-Chloro-5-hydroxy-6-methylpyridine, C-60099
2-Chloro-3-methoxypyridine, *in* C-60100
3-Chloro-5-methoxypyridine, *in* C-60102

$C_6H_6ClNO_2$
6-Chloro-4-methoxy-2(1*H*)-pyridinone, *in* C-70074

$C_6H_6ClNO_2S$
3-Chloro-2-(methylsulfonyl)pyridine, *in* C-60129

C_6H_6ClNS
3-Chloro-2-(methylthio)pyridine, *in* C-60129

$C_6H_6Cl_2O$
2,4-Dichloro-3,4-dimethyl-2-cyclobuten-1-one, D-60130
4,4-Dichloro-2,3-dimethyl-2-cyclobuten-1-one, D-60131

C_6H_6FNS
2-Amino-3-fluorobenzenethiol, A-80073
2-Amino-5-fluorobenzenethiol, A-80074
2-Amino-6-fluorobenzenethiol, A-80075
4-Amino-2-fluorobenzenethiol, A-80076
4-Amino-3-fluorobenzenethiol, A-80077

$C_6H_6F_2O_4$
Difluoromaleic acid; Di-Me ester, *in* D-80159

$C_6H_6F_4O_4$
Tetrafluorobutanedioic acid; Di-Me ester, *in* T-80049

C_6H_6INO
3-Hydroxy-2-iodo-6-methylpyridine, H-60159

$C_6H_6I_2S$
2,5-Bis(iodomethyl)thiophene, B-80153

$C_6H_6N_2$
1,4-Dihydropyrrolo[3,2-*b*]pyrrole, D-30286
2-Methyl-4-cyanopyrrole, *in* M-60125
2-Methylenepentanedinitrile, M-80089

$C_6H_6N_2O$
2-Acetylpyrimidine, A-60044
4-Acetylpyrimidine, A-60045
5-Acetylpyrimidine, A-60046
4-Cyano-2,5-dimethyloxazole, *in* D-80461
1,4-Dihydrofuro[3,4-*d*]pyridazine, D-60241

$C_6H_6N_2OS_2$
3-Mercapto-6(1*H*)-pyridazinethione; *S*-Ac, *in* M-80028

$C_6H_6N_2O_2$
5-Acetyl-2(1*H*)-pyrimidinone, A-60048
▷ 1,4-Benzoquinone; Dioxime, *in* B-70044
Ethyl dicyanoacetate, *in* D-70149
▷ 1-Hydroxy-2-phenyldiazene 2-oxide, H-70208
3-Methyl-4-nitropyridine, M-70099
▷ Urocanic acid, U-70005

$C_6H_6N_2O_3$
5-Acetyl-2,4(1*H*,3*H*)-pyrimidinedione, A-60047
3,4-Diacetylfurazan, D-80045
4-Methoxy-3-nitropyridine, *in* N-70063
▷ 3-Methyl-4-nitropyridine; *N*-Oxide, *in* M-70099
3-Nitro-4(1*H*)-pyridone; *N*-Me, *in* N-70063

$C_6H_6N_2O_4$
3,6-Diacetyl-1,4,2,5-dioxadiazine, D-80044
▷ 3,4-Diacetylfuroxan, *in* D-80045
1*H*-Pyrazole-4,5-dicarboxylic acid; 1-Me, *in* P-80199
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidineacetic acid, T-70060

$C_6H_6N_2S$
1,4-Dihydrothieno[3,4-*d*]pyridazine, D-60289

$C_6H_6N_2S_2$
[Bis(methylthio)methylene]propanedinitrile, *in* D-60395
1,4-Dithiocyano-2-butene, D-60510

$C_6H_6N_4$
7-Amino-3*H*-imidazo[4,5-*b*]pyridine, A-80087
4-Amino-1*H*-imidazo[4,5-*c*]pyridine, A-70161
2,2′-Bi-1*H*-imidazole, B-60107
1,3(5)-Bi-1*H*-pyrazole, B-60119
1*H*-Pyrazolo[3,4-*d*]pyrimidine; 1-Me, *in* P-70156

$C_6H_6N_4O$
3-Amino-1*H*-pyrazole-4-carboxylic acid; Nitrile, *N*(3)-Ac, *in* A-70187
2-Aminopyrrolo[2,3-*d*]pyrimidin-4-one, A-60255
1,3-Dihydro-1-methyl-2*H*-imidazo[4,5-*b*]pyrazin-2-one, *in* I-60006
Imidazo[2,1-*c*][1,2,4]triazin-4(1*H*)-one; 1-Me, *in* I-80007
Imidazo[2,1-*c*][1,2,4]triazin-4(1*H*)-one; 2-Me, *in* I-80007
Imidazo[2,1-*c*][1,2,4]triazin-4(1*H*)-one; 8-Me, *in* I-80007
1*H*-Pyrazolo[3,4-*d*]pyrimidine; 1-Me, 5-oxide, *in* P-70156
Pyrazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one; 1-Me, *in* P-80201
Pyrazolo[5,1-*c*][1,2,4]triazin-4(1*H*)-one; 2-Me, *in* P-80201

$C_6H_6N_4O_2$
3,9-Dihydro-9-methyl-1*H*-purine-2,6-dione, D-60257

$C_6H_6N_4O_4$
1,2,4,5-Tetrazine-3,6-dicarboxylic acid; Di-Me ester, *in* T-80163

$C_6H_6N_4S$
2-Aminopyrrolo[2,3-*d*]pyrimidine-4-thione, A-80144
1,3-Dihydro-1-methyl-2*H*-imidazo[4,5-*b*]pyrazine-2-thione, *in* D-60247
1,7-Dihydro-6*H*-purine-6-thione; 1-Me, *in* D-60270
1,7-Dihydro-6*H*-purine-6-thione; 3-Me, *in* D-60270
1,7-Dihydro-6*H*-purine-6-thione; 7-Me, *in* D-60270
1,7-Dihydro-6*H*-purine-6-thione; 9-Me, *in* D-60270
▷ 6-Mercaptopurine; *S*-Me, *in* D-60270
2-(Methylthio)-1*H*-imidazo[4,5-*b*]pyrazine, *in* D-60247
6-(Methylthio)-5*H*-imidazo[4,5-*c*]pyridazine, *in* D-70215

$C_6H_6N_6$
2,4-Diaminopteridine, D-60042
4,6-Diaminopteridine, D-60043
4,7-Diaminopteridine, D-60044
6,7-Diaminopteridine, D-60045

$C_6H_6N_6O_2$
2,6-Diamino-4,7(3*H*,8*H*)-pteridinedione, D-60047
2,7-Diamino-4,6(3*H*,5*H*)-pteridinedione, D-60046
2,4-Diaminopteridine; 5,8-Dioxide, *in* D-60042

$C_6H_6N_6O_3$
1,3,5-Triazine-2,4,6-tricarboxaldehyde; Trioxime, *in* T-60237

C_6H_6O
4,5-Dihydrocyclobuta[*b*]furan, D-60212

C_6H_6OS
2-Methyl-3-thiophenecarboxaldehyde, M-70139
3-Methyl-2-thiophenecarboxaldehyde, M-70140
4-Methyl-2-thiophenecarboxaldehyde, M-70141
4-Methyl-3-thiophenecarboxaldehyde, M-70142
5-Methyl-2-thiophenecarboxaldehyde, M-70143
5-Methyl-3-thiophenecarboxaldehyde, M-70144

$C_6H_6O_2$
3-Furanacetaldehyde, F-60083
1,5-Hexadiene-3,4-dione, H-60039
3-Hexyne-2,5-dione, H-70090
2-Methylene-1,3-cyclopentanedione, M-80083
2-Oxiranylfuran, O-70078
3-Oxo-1-cyclopentenecarboxaldehyde, O-60062

$C_6H_6O_2S$
3-Acetoxythiophene, *in* T-60212
2-(Hydroxyacetyl)thiophene, H-70103

$C_6H_6O_3$
▷ 5-Hydroxymethyl-2-furancarboxaldehyde, H-70177
2-Methylene-3-oxocyclobutanecarboxylic acid, M-80088
4-Oxo-2-butynoic acid; Et ester, *in* O-80070
2-Propenoic acid; Anhydride, *in* P-70121

$C_6H_6O_4$
3-Acetyl-4-hydroxy-2(5*H*)-furanone, A-60030
1,2,3,4-Benzenetetrol, B-60014
Dimethylenebutanedioic acid, D-70409

$C_6H_6O_5$
(2-Oxopropylidene)propanedioic acid, O-70100

$C_6H_6O_6$
▷ Aconitic acid, A-70055

C_6H_6S
2,3-Dihydro-2,3-dimethylenethiophene, D-70195
3-Vinylthiophene, V-80010

$C_6H_7BrO_2$
2-Bromo-1,3-cyclohexanedione, B-70201

C_6H_7ClO
2-Chloro-2-cyclohexen-1-one, C-60050
2-Chloro-3-methyl-2-cyclopenten-1-one, C-70090
5-Chloro-3-methyl-2-cyclopenten-1-one, C-70091
3,5-Hexadienoic acid; Chloride, *in* H-70038
5-Hexynoic acid; Chloride, *in* H-80086

$C_6H_7ClO_2$
2-Chloro-1,3-cyclohexanedione, C-80046

$C_6H_7ClO_4$
▷ Chloromaleic acid; Di-Me ester, *in* C-80043

$C_6H_7IN_2$
2-Amino-3-iodopyridine; N-Me, *in* A-80088

$C_6H_7IN_2O_2$
6-Iodo-1,3-dimethyluracil, *in* I-70057

C_6H_7N
1-Cyano-3-methylbicyclo[1.1.0]butane, *in* M-70053
5-Cyano-1-pentyne, *in* H-80086
2-Vinyl-1*H*-pyrrole, V-60013

C_6H_7NO
3-Acetylpyrrole, A-70052
2-Cyanocyclopentanone, *in* O-70084
1,2-Dihydro-3*H*-azepin-3-one, D-70171
5-Methyl-1*H*-pyrrole-2-carboxaldehyde, M-70129
4-(2-Propynyl)-2-azetidinone, P-60185

C_6H_7NOS
2-Acetyl-3-aminothiophene, A-70029
2-Pyridinethiol; *S*-Me, *N*-Oxide, *in* P-60223
2-Pyrrolethiolcarboxylic acid; Me ester, *in* P-80226

$C_6H_7NO_2$
1-Acetyl-1,2-dihydro-3*H*-pyrrol-3-one, *in* D-70262
3-Amino-1,2-benzenediol, A-70089
▷ 4-Amino-1,2-benzenediol, A-70090
1-Azabicyclo[3.2.0]heptane-2,7-dione, A-60330
1-Azabicyclo[3.2.0]heptane-2,7-dione, A-70273
3,4-Dimethyl-1*H*-pyrrole-2,5-dione, D-80474

3-Hydroxy-2-methyl-4(1*H*)-pyridinone, H-80214
3-Hydroxy-2(1*H*)-pyridinone; *N*-Me, *in* H-60223
3-Hydroxy-4(1*H*)-pyridinone; *N*-Me, *in* H-60227
4-Hydroxy-2(1*H*)-pyridinone; *N*-Me, *in* H-60224
5-Hydroxy-2(1*H*)-pyridinone; *N*-Me, *in* H-60225
6-Hydroxy-2(1*H*)-pyridinone; *N*-Me, *in* H-60226
3-Methoxy-4(1*H*)-pyridinone, *in* H-60227
6-Methoxy-2(1*H*)-pyridinone, *in* H-60226
Methyl 1-cyanocyclopropanecarboxylate, *in* C-80196
5-Methyl-1*H*-pyrrole-2-carboxylic acid, M-60124
5-Methyl-1*H*-pyrrole-3-carboxylic acid, M-60125
1-Nitro-1,3-cyclohexadiene, N-70047
4-Oxo-2-butynoic acid; Dimethylamide, *in* O-80070

$C_6H_7NO_3$
2,5-Dimethyl-4-oxazolecarboxylic acid, D-80461
5-Hydroxymethyl-2-furancarboxaldehyde; Oxime, *in* H-70177
5-Isoxazolecarboxylic acid; Et ester, *in* I-60142
4-Methoxy-1*H*-pyrrole-3-carboxylic acid, *in* H-80250
4-Methoxy-2-pyrrolecarboxylic acid, *in* H-80249
3-Oxo-2-azabicyclo[2.1.1]hexane-1-carboxylic acid, O-80057

C_6H_7NS
▷ 2-Pyridinethiol; *S*-Me, *in* P-60223
▷ 2(1*H*)-Pyridinethione; *N*-Me, *in* P-60224
4(1*H*)-Pyridinethione; *N*-Me, *in* P-60225

$C_6H_7NS_2$
4-(Methylthio)-2(1*H*)-pyridinethione, *in* M-80029
4-(Methylthio)-2(1*H*)-pyridinethione, *in* P-60219

C_6H_7NSe
2-(Methylseleno)pyridine, *in* P-70170
2(1*H*)-Pyridineselone; *N*-Me, *in* P-70170

$C_6H_7N_3$
2-Amino-5-vinylpyrimidine, A-60269

$C_6H_7N_3OS_2$
5-Amino-2-thiazolecarbothioamide; N^5-Ac, *in* A-60260
5-Amino-4-thiazolecarbothioamide; N^5-Ac, *in* A-60261

$C_6H_7N_5$
6-Amino-7-methylpurine, A-60226
2-(Methylamino)purine, *in* A-60243
8-(Methylamino)purine, *in* A-60244
9-Methyl-9*H*-purin-8-amine, *in* A-60244

$C_6H_7N_5O$
6-Amino-1,3-dihydro-1-methyl-2*H*-purine-2-one, *in* A-60144
2,6-Diamino-1,5-dihydro-4*H*-imidazo[4,5-*c*]pyridin-4-one, D-60034

$C_6H_7N_7$
2,4,7-Triaminopteridine, T-60229
4,6,7-Triaminopteridine, T-60230

C_6H_8
2-Methylenebicyclo[2.1.0]pentane, M-80075

$C_6H_8Cl_2N_2$
3-Chloro-6-methylpyridazine; 2-Methochloride, *in* C-70112

$C_6H_8Cl_2O_3$
3,3′-Oxybispropanoic acid; Dichloride, *in* O-80098

$C_6H_8F_4$
1,1,2,2-Tetrafluoro-3,4-dimethylcyclobutane, T-60047

$C_6H_8F_6O_6S_4$
1,4-Dithioniabicyclo[2.2.0]hexane; Bis(trifluoromethanesulfonate), *in* D-70527

$C_6H_8N_2$
▷ 2-(Aminomethyl)pyridine, A-60227
3-(Aminomethyl)pyridine, A-60228
4-(Aminomethyl)pyridine, A-60229
4,5-Dimethylpyrimidine, D-70436
3,4,5,6-Tetrahydro-4,5-bis(methylene)pyridazine, T-60062
1,4,5,6-Tetrahydrocyclopentapyrazole, T-80055

$C_6H_8N_2O$
2-Amino-3-hydroxy-6-methylpyridine, A-60192
5-Amino-3-hydroxy-2-methylpyridine, A-60193
2-Amino-4-methoxypyridine, *in* A-60253
2-Amino-6-methoxypyridine, *in* A-60252
3-Amino-2-methoxypyridine, *in* A-60249
3-Amino-4-methoxypyridine, *in* A-60254
4-Amino-2-methoxypyridine, *in* A-60250
5-Amino-2-methoxypyridine, *in* A-60251
3-Amino-1-methyl-2(1*H*)-pyridinone, *in* A-60249
3-Amino-1-methyl-4(1*H*)-pyridinone, *in* A-60254
5-Amino-1-methyl-2(1*H*)-pyridinone, *in* A-60251
6-Amino-1-methyl-2(1*H*)-pyridinone, *in* A-60252
Bis(2-cyanoethyl)ether, *in* O-80098
2,3-Dihydro-1,6-dimethyl-3-oxopyridazinium hydroxide, inner salt, *in* M-70124
4,5-Dimethylpyrimidine; 1-Oxide, *in* D-70436
4,5-Dimethylpyrimidine; 3-Oxide, *in* D-70436
7-Hydroxy-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazole, H-60118
3-Methoxy-6-methylpyridazine, *in* M-70124
6-Methyl-3-pyridazinone; 2-Me, *in* M-70124
5-Methyl-1*H*-pyrrole-2-carboxaldehyde; Oxime, *in* M-70129

$C_6H_8N_2OS$
4,5,6,7-Tetrahydrobenzothiadiazole; 2-Oxide, *in* T-70042

$C_6H_8N_2O_2$
2,5-Dimethyl-4-oxazolecarboxylic acid; Amide, *in* D-80461
5-Ethyl-2,4(1*H*,3*H*)-pyrimidinedione, E-60054
3-Hydroxy-6-methylpyridazine; Me ether, 1-Oxide, *in* M-70124
1*H*-Imidazole-4-carboxylic acid; Et ester, *in* I-60004
4,5,6,7-Tetrahydroisoxazolo[4,5-*c*]pyridin-3-ol, T-60071
4,5,6,7-Tetrahydroisoxazolo[5,4-*c*]pyridin-3-ol, T-60072
Tetrahydro-1*H*,5*H*-pyrazolo[1,2-*a*]pyrazole-1,5-dione, T-70087

$C_6H_8N_2O_3S$
4,5,6,7-Tetrahydrobenzothiadiazole; 1,1,2-Trioxide, *in* T-70042

$C_6H_8N_2O_4$
1,2-Dinitrocyclohexene, D-70451

$C_6H_8N_2S$
4,6-Dimethyl-2(1*H*)-pyrimidinethione, D-60450
4-Methylthio-2-pyridinamine, *in* A-80139
4-Methylthio-3-pyridinamine, *in* A-80140
6-Methylthio-2-pyridinamine, *in* A-80142
6-Methylthio-3-pyridinamine, *in* A-80141
4,5,6,7-Tetrahydrobenzothiadiazole, T-70042

$C_6H_8N_2S_2$
3,6-Bis(methylthio)pyridazine, *in* M-80028
1,4-Diamino-2,3-benzenedithiol, D-60030
2,5-Diamino-1,4-benzenedithiol, D-70035
3,6-Diamino-1,2-benzenedithiol, D-70036
2-Methyl-6-(methylthio)-3(2*H*)-pyridazinethione, *in* M-80028

$C_6H_8N_2S_4$
1,4-Diamino-2,3,5,6-benzenetetrathiol, D-60031

$C_6H_8N_4O_4$
3,4-Diacetylfuroxan dioxime, *in* D-80045
5-Nitrohistidine, N-60028
Schmitz's compound, *in* D-80044
Tetrahydro-1,2,4,5-tetrazine-3,6-dione; 1,5-Di-Ac, *in* T-70097

$C_6H_8N_6O_2$
3,6-Diamino-1,2,4,5-tetrazine; Di-*N*-Ac, *in* D-70045
3,6-Pyridazinedicarboxylic acid; Dihydrazide, *in* P-70168

C_6H_8O
Bicyclo[3.1.0]hexan-2-one, B-60088
3-Cyclohexen-1-one, C-60211
2,3-Dimethyl-2-cyclobuten-1-one, D-60415
1-Hexen-5-yn-3-ol, H-70089
2-Methylene-4-pentenal, M-70074
3-Methylene-4-penten-2-one, M-70075
7-Oxabicyclo[2.2.1]hept-2-ene, O-70054
7-Oxabicyclo[4.1.0]hept-3-ene, O-60047
2-Oxatricyclo[4.1.$0^{1,6}$.$0^{3,5}$]heptane, O-60052
Tetrahydro-3,4-bis(methylene)furan, T-70046

C_6H_8OS
2-Methyl-3-furanthiol; *S*-Me, *in* M-70082
3-Methyl-2-thiophenemethanol, M-80176
4-Methyl-2-thiophenemethanol, M-80177
5-Methyl-2-thiophenemethanol, M-80178
2-Thiabicyclo[2.2.1]heptan-3-one, T-60186
2-Thiabicyclo[2.2.1]hept-5-ene; *endo*-2-Oxide, *in* T-70160
2-Thiabicyclo[2.2.1]hept-5-ene; *exo*-2-Oxide, *in* T-70160
1-(2-Thienyl)ethanol, T-80178
1-(3-Thienyl)ethanol, T-80179
3-Thiopheneethanol, T-60211

$C_6H_8O_2$
Bicyclo[1.1.1]pentane-1-carboxylic acid, B-60101
Dihydro-4-methyl-3-methylene-2(3*H*)-furanone, D-80222
5,6-Dihydro-3-methyl-2*H*-pyran-2-one, D-80228
5,6-Dihydro-4-methyl-2*H*-pyran-2-one, *in* H-80211
3,4-Dihydro-2*H*-pyran-5-carboxaldehyde, D-70252
Dihydro-3-vinyl-2(3*H*)-furanone, D-70279
3,3-Dimethyl-1-cyclopropene-1-carboxylic acid, D-60417
3,4-Dimethyl-2(5*H*)-furanone, D-60423
3,4-Hexadienoic acid, H-70037
3,5-Hexadienoic acid, H-70038
2-Hexenedial, H-80079
3-Hexenedial, H-80080
3-Hexene-2,5-dione, H-80084
5-Hexynoic acid, H-80086
▷ 2-Hydroxy-3-methyl-2-cyclopenten-1-one, H-60174
4-Hydroxy-2-methyl-2-cyclopenten-1-one, H-60175
5-(Hydroxymethyl)-2-cyclopenten-1-one, H-80199
3-Hydroxymethyl-2-methylfuran, H-80207
3-Methylbicyclo[1.1.0]butane-1-carboxylic acid, M-70053
2-Methylenecyclopropaneacetic acid, M-70067
3-Methyl-4-oxo-2-pentenal, M-70104
3-Oxabicyclo[3.2.0]heptan-2-one, O-70053
4-Pentynoic acid; Me ester, *in* P-80062
Tetrahydro-6-methylene-2*H*-pyran-2-one, T-70074

$C_6H_8O_2S$
2-Thiabicyclo[2.2.1]hept-5-ene; 2,2-Dioxide, *in* T-70160
3-Thiatricyclo[2.2.1.$0^{2,6}$]heptane; *S*,*S*-Dioxide, *in* T-70165

$C_6H_8O_3$
2,5-Bis(hydroxymethyl)furan, B-60160
3,4-Bis(hydroxymethyl)furan, B-60161
2-Cyclopropyl-2-oxoacetic acid; Me ester, *in* C-60231
Dihydro-4,4-dimethyl-2,3-furandione, D-70196

4,5-Dihydro-3-(methoxymethylene)-2(3*H*)-furanone, D-70222
3,6-Dihydro-2*H*-pyran-2-carboxylic acid, D-80242
5,5-Dimethyl-4-methylene-1,2-dioxolan-3-one, D-60428
4-Ethoxy-2(5*H*)-furanone, *in* F-80087
4-Hydroxy-2,5-dimethyl-3(2*H*)-furanone, H-60120
5-Hydroxymethyl-4-methyl-2(5*H*)-furanone, H-60187
2-Oxocyclopentanecarboxylic acid, O-70084
4-Oxo-2-hexenoic acid, O-80082
5-Oxo-3-hexenoic acid, O-70092
5-Oxo-3-hexenoic acid, O-80083
6-Oxo-4-hexenoic acid, O-80084
4-Oxo-2-pentenoic acid; Me ester, *in* O-70098

$C_6H_8O_3S_2$
2-Thiophenesulfonic acid; Et ester, *in* T-60213

$C_6H_8O_4$
Ethyl diformylacetate, *in* D-60190
2-Hydroxy-2-(hydroxymethyl)-2*H*-pyran-3(6*H*)-one, H-70141

C_6H_8S
2-Thiabicyclo[2.2.1]hept-5-ene, T-70160
3-Thiatricyclo[2.2.1.0^{2,6}]heptane, T-70165

$C_6H_8S_3$
2,5-Thiophenedimethanethiol, T-70184

C_6H_9Br
1-Bromo-3,3-dimethyl-1-butyne, B-70207
2-Bromo-1,5-hexadiene, B-70216
1-Bromo-1-hexyne, B-70218
1-Bromo-2-hexyne, B-70219

$C_6H_9BrO_2$
2-Bromomethyl-2-propenoic acid; Et ester, *in* B-70249

C_6H_9Cl
2-Chloro-1,5-hexadiene, C-70070

C_6H_9FO
2-Fluorocyclohexanone, F-60021

$C_6H_9F_3O$
1,1,1-Trifluoro-3,3-dimethyl-2-butanone, T-80272

$C_6H_9F_3O_2$
Trifluoroacetic acid; *tert*-Butyl ester, *in* T-80267

C_6H_9I
1-Iodocyclohexene, I-70026
1-Iodo-1-hexyne, I-70040

C_6H_9IO
2-Iodocyclohexanone, I-60042
6-Iodo-5-hexyn-1-ol, I-70041

C_6H_9N
2-Cyano-1,1-dimethylcyclopropane, *in* D-80444
3-Ethyl-1*H*-pyrrole, E-80067

C_6H_9NO
3-Amino-2-cyclohexen-1-one, A-70125
3-Cyclohexen-1-one; Oxime, *in* C-60211
1,2-Dihydro-2,2-dimethyl-3*H*-pyrrol-3-one, D-60230
3,4-Dihydro-6-methyl-2(1*H*)-pyridinone, D-80229
3-Methylbicyclo[1.1.0]butane-1-carboxylic acid; Amide, *in* M-70053
4-(2-Propenyl)-2-azetidinone, *in* A-60172

$C_6H_9NO_2$
3-(1-Aminocyclopropyl)-2-propenoic acid, A-60123
4-Amino-2,5-hexadienoic acid, A-60166
3,6-Dihydro-2*H*-pyran-2-carboxylic acid; Amide, *in* D-80242
3,4-Dihydro-2*H*-pyrrole-5-carboxylic acid; Me ester, *in* D-80249
Hexahydro-2*H*-furo[3,2-*b*]pyrrol-2-one, H-80059
3-Methyl-1-nitrocyclopentene, M-80122
▷ 2-Pyrrolidinone; *N*-Ac, *in* P-70188
1,2,3,6-Tetrahydro-3-pyridinecarboxylic acid, T-60084
3,4,4-Trimethyl-5(4*H*)-isoxazolone, T-60367

$C_6H_9NO_3$
3-Aminodihydro-2(3*H*)-furanone; *N*-Ac, *in* A-60138
2-Amino-2-(hydroxymethyl)-4-pentynoic acid, A-60191
3-*tert*-Butyl-1,4,2-dioxazol-5-one, B-80286
Methyl 2-formyl-3-methylamino-2 propenoate, *in* A-80134
2,3-Morpholinedione; N-Et, *in* M-80193
2-Nitrocyclohexanone, N-80043
4-Oxo-2-piperidinecarboxylic acid, O-60089
5-Oxo-2-pyrrolidinecarboxylic acid; Me ester, *in* O-70102
1,2,3,6-Tetrahydro-3-hydroxy-2-pyridinecarboxylic acid, T-60068
1,2,5,6-Tetrahydro-5-hydroxy-3-pyridinecarboxylic acid, T-70065

$C_6H_9NO_3S$
5-Oxo-3-thiomorpholinecarboxylic acid; Me ester, *in* O-80095

$C_6H_9NO_4$
2-Amino-3-methylenepentanedioic acid, A-60219

$C_6H_9NO_6$
O-Oxalylhomoserine, *in* A-70156

$C_6H_9NS_2$
2(3*H*)-Thiazolethione; *S*-Isopropyl, *in* T-60200

$C_6H_9N_3O$
2-Amino-6-methyl-4(1*H*)-pyrimidinone; 2-*N*-Me, *in* A-60230

$C_6H_9N_3O_2$
2-Amino-4(5)-imidazoleacetic acid; Me ester, *in* A-80086
α-Amino-1*H*-imidazole-1-propanoic acid, A-60204
α-Amino-1*H*-imidazole-2-propanoic acid, A-60205
3-Amino-5-methyl-1*H*-pyrazole-4-carboxylic acid; Me ester, *in* A-80110
3-Amino-1*H*-pyrazole-4-carboxylic acid; Et ester, *in* A-70187
4-Amino-1*H*-pyrazole-3-carboxylic acid; Et ester, *in* A-70189
3-Amino-1*H*-pyrazole-5-carboxylic acid; *N*(1)-Me, Me ester, *in* A-70188
5-Amino-1*H*-pyrazole-3-carboxylic acid; *N*(1)-Me, Me ester, *in* A-70191
▷ Cupferron, *in* H-70208
2,4-Dimethoxy-6-methyl-1,3,5-triazine, *in* M-60132
3,4-Dimethyl-1*H*-pyrrole-2,5-dione; Dioxime, *in* D-80474
4-Methoxy-1,6-dimethyl-1,3,5-triazin-2(1*H*)-one, *in* M-60132
1*H*-1,2,3-Triazole-4-carboxylic acid; 1-Me, Et ester, *in* T-60239
1*H*-1,2,3-Triazole-4-carboxylic acid; 2-Me, Et ester, *in* T-60239
1,3,6-Trimethyl-5-azauracil, *in* M-60132

$C_6H_9N_3O_2S$
5-Mercaptohistidine, M-80025

$C_6H_9N_3O_3$
Aconitic acid; Triamide, *in* A-70055
Hexahydro-1,3,5-triazine; 1,3,5-Triformyl, *in* H-60060
Trimethyl isocyanurate, *in* C-60179

$C_6H_{10}Br_4$
2,3-Bis(bromomethyl)-1,4-dibromobutane, B-60144

$C_6H_{10}ClF_2NO_2$
2-Amino-4-chloro-4,4-difluorobutanoic acid; Et ester, *in* A-60107

$C_6H_{10}ClNO_2$
1-Chloro-1-nitrocyclohexane, C-70131

$C_6H_{10}ClNO_3$
2-Amino-5-chloro-6-hydroxy-4-hexenoic acid, A-60110

$C_6H_{10}Cl_3N$
1,1,2-Trichloro-2-(diethylamino)ethylene, T-70222

$C_6H_{10}Cl_4$
2,3-Bis(chloromethyl)-1,4-dichlorobutane, B-60148

$C_6H_{10}INO$
6-(Iodomethyl)-2-piperidinone, I-80036

$C_6H_{10}N_2$
2-Amino-5-hexenoic acid; Nitrile, *in* A-60169
3-Amino-2-hexenoic acid; Nitrile, *in* A-60170
Azocyclopropane, A-80205

$C_6H_{10}N_2O$
Azoxycyclopropane, *in* A-80205

$C_6H_{10}N_2O_2$
5-Amino-3,4-dihydro-2*H*-pyrrole-2-carboxylic acid; Me ester, *in* A-70135
2,5-Dihydro-4,6-dimethoxypyrimidine, *in* D-70256
Dihydro-4,4-dimethyl-2,3-furandione; Hydrazone, *in* D-70196
1-Dimethylamino-4-nitro-1,3-butadiene, D-70367

$C_6H_{10}N_2O_3$
2-Amino-3-methylenepentanedioic acid; 5-Amide, *in* A-60219
3-Piperidinecarboxylic acid; *N*-Nitroso, *in* P-70102

$C_6H_{10}N_2O_4$
2,5-Piperazinedicarboxylic acid, P-60157

$C_6H_{10}N_4$
1,2,3,5-Tetraaminobenzene, T-60012
1,2,4,5-Tetraaminobenzene, T-60013

$C_6H_{10}N_4O$
4-Amino-1,3,5-triazin-2(1*H*)-one; 1,4,4-*N*-Tri-Me, *in* A-80149

$C_6H_{10}N_4O_2$
Tetrahydroimidazo[4,5-*d*]imidazole-2,5(1*H*,3*H*)-dione; 1,4-Di-Me, *in* T-70066
Tetrahydroimidazo[4,5-*d*]imidazole-2,5(1*H*,3*H*)-dione; 1,6-Di-Me, *in* T-70066

$C_6H_{10}N_4S$
1-(4,5-Dihydro-1*H*-imidazol-2-yl)-2-imidazolidinethione, D-60246

$C_6H_{10}O$
Bicyclo[2.1.1]hexan-2-ol, B-70100
tert-Butoxyethyne, *in* E-80070
2,3-Dihydro-4,5-dimethylfuran, D-80190
3,5-Hexadien-1-ol, H-70039
▷ 2-Hexenal, H-60076
1-Methyl-6-oxabicyclo[3.1.0]hexane, M-80126
▷ 2-Methyl-2-pentenal, M-70106
4-Methyl-4-pentenal, M-80134

$C_6H_{10}OS$
2,3-Dihydro-4,5-dimethylthiophene; 1-Oxide, *in* D-80195
2-Mercaptocyclohexanone, M-70025
3-Mercaptocyclohexanone, M-70026
4-Mercaptocyclohexanone, M-70027
2-(Methylthio)cyclopentanone, M-70136
2-Oxepanethione, O-70077
4-Thioxo-2-hexanone, T-60215

$C_6H_{10}O_2$
2-Cyclohexene-1,4-diol, C-80181
4-Cyclohexene-1,2-diol, C-80182
Dihydro-4,5-dimethyl-2(3*H*)-furanone, D-80191
2,3-Dimethyl-3-butenoic acid, D-80438
2,2-Dimethylcyclopropanecarboxylic acid, D-80444
2,2-Dimethyl-4-methylene-1,3-dioxolane, D-70419
▷ 1,5-Hexadiene-3,4-diol, H-70036
2-Hexyne-1,6-diol, H-80085
2-Methoxycyclopentanone, *in* H-60114
4-Methoxy-3-penten-2-one, *in* P-60059
4-Oxohexanal, O-60073
5-Oxohexanal, O-70091
Tetrahydro-4-methyl-2*H*-pyran-2-one, *in* H-70182

$C_6H_{10}O_2S$
3-(Acetylthio)cyclobutanol, *in* M-60019
2,5-Dihydro-2,5-dimethylthiophene; 1,1-Dioxide, *in* D-60233
O-Ethyl 3-oxobutanethioate, *in* O-70080
S-Ethyl 3-oxobutanethioate, *in* O-70080
3-Mercaptocyclopentanecarboxylic acid, M-60021

$C_6H_{10}O_3$
2,2-Dimethyl-1,3-dioxolane-4-carboxaldehyde, D-70400
Epiverrucarinolactone, *in* D-60353
2-Ethoxy-2-propenoic acid; Me ester, *in* E-70037
4-Hydroxy-2-butenoic acid; Et ester, *in* H-80134
5-Hydroxy-3-methyl-2-pentenoic acid, H-80211
6-(Hydroxymethyl)tetrahydro-2*H*-pyran-2-one, *in* D-60329
▷ 3-Methyloxiranecarboxylic acid; Et ester, *in* M-80127
▷ 3-Methyloxiranecarboxylic acid; Et ester, *in* M-80127
3-Methyl-2-oxobutanoic acid; Me ester, *in* M-80129
5-Oxopentanoic acid; Me ester, *in* O-80089
3-Oxopropanoic acid; Isopropyl ester, *in* O-60090
3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2*H*-pyran-2-one, T-60067
Tetrahydro-3-hydroxy-4-methyl-2*H*-pyran-2-one, *in* D-60353

$C_6H_{10}O_4$
4-Hydroxy-3,3-dimethyl-2-oxobutanoic acid, H-60124
Methylpropanedioic acid; Di-Me ester, *in* M-80149
1,3,7,9-Tetraoxaspiro[4,5]decane, T-60163
1,4,6,10-Tetraoxaspiro[4,5]decane, T-60164

$C_6H_{10}O_5$
▷ Diethyl dicarbonate, *in* D-70111
Methyl hydrogen 3-hydroxyglutarate, M-70089
3,3′-Oxybispropanoic acid, O-80098

$C_6H_{10}O_6$
Dimethyl tartrate, *in* T-70005

$C_6H_{10}O_{12}P_2$
myo-Inositol; 1,4-Diphosphate, *in* I-80015

$C_6H_{10}S$
2,3-Dihydro-2,2-dimethylthiophene, D-60232
2,3-Dihydro-4,5-dimethylthiophene, D-80195
2,5-Dihydro-2,5-dimethylthiophene, D-60233

$C_6H_{10}S_4$
2,2′-Bi-1,3-dithiolane, B-60103
Di-2-propenyl tetrasulfide, D-80515
Hexahydro-1,4-dithiino[2,3-*b*]-1,4-dithiin, H-60051

$C_6H_{11}Br$
1-Bromo-3-hexene, B-80209
5-Bromo-1-hexene, B-60263
6-Bromo-1-hexene, B-60264
(Bromomethyl)cyclopentane, B-70241
5-Bromo-3-methyl-1-pentene, B-60299

$C_6H_{11}BrO$
5-Bromo-2-hexanone, B-60262
1-Bromo-4-methyl-2-pentanone, B-60298

$C_6H_{11}BrO_2$
2-Bromo-4-methylpentanoic acid, B-70248

$C_6H_{11}Br_2NO_2$
6-Amino-2,2-dibromohexanoic acid, A-60124

$C_6H_{11}Cl$
6-Chloro-1-hexene, C-80058
5-Chloro-3-methyl-1-pentene, C-60117

$C_6H_{11}ClFNO_2$
2-Amino-4-chloro-4-fluorobutanoic acid; Et ester, *in* A-60108

$C_6H_{11}ClO$
2-Chloro-1-hexen-3-ol, C-80059
2-Chloro-4-hexen-3-ol, C-80060
4-Chloro-4-hexen-3-ol, C-80061
6-Chloro-2-hexen-1-ol, C-80062
6-Chloro-3-hexen-1-ol, C-80063
6-Chloro-4-hexen-1-ol, C-80064
6-Chloro-5-hexen-3-ol, C-80065

$C_6H_{11}Cl_2NO_2$
6-Amino-2,2-dichlorohexanoic acid, A-60126

$C_6H_{11}F_2NO_2$
2-Amino-3,3-difluorobutanoic acid; Et ester, *in* A-60133

$C_6H_{11}I$
1-Iodo-1-hexene, I-70037
6-Iodo-1-hexene, I-70038
(Iodomethyl)cyclopentane, I-70047

$C_6H_{11}IO$
1-Iodo-3,3-dimethyl-2-butanone, I-60044
6-Iodo-5-hexen-1-ol, I-70039

$C_6H_{11}N$
2-Aminobicyclo[2.1.1]hexane, A-70095
3,4-Dihydro-2,2-dimethyl-2*H*-pyrrole, D-60229
3-Isocyanopentane, I-80059

$C_6H_{11}NO$
3,4-Dihydro-2,2-dimethyl-2*H*-pyrrole; *N*-Oxide, *in* D-60229
2,2-Dimethylcyclopropanecarboxylic acid; Amide, *in* D-80444
5-Ethoxy-3,4-dihydro-2*H*-pyrrole, *in* P-70188
2-Oxa-3-azabicyclo[2.2.2]octane, O-70051
1-Oxa-2-azaspiro[2,5]octane, O-70052

$C_6H_{11}NOS$
3-Mercaptocyclopentanecarboxylic acid; Amide, *in* M-60021

$C_6H_{11}NO_2$
2-Amino-2-ethyl-3-butenoic acid, A-60150
1-Amino-2-ethylcyclopropanecarboxylic acid, A-60151
2-Amino-2-hexenoic acid, A-60167
2-Amino-3-hexenoic acid, A-60168
2-Amino-5-hexenoic acid, A-60169
3-Amino-2-hexenoic acid, A-60170
3-Amino-4-hexenoic acid, A-60171
3-Amino-5-hexenoic acid, A-60172
6-Amino-2-hexenoic acid, A-60173
2-Amino-3-methyl-3-butenoic acid; Me ester, *in* A-60218
4,4-Dimethoxybutanenitrile, *in* O-80068
2,6-Dimethyl-3-morpholinone, D-80454
2-Methyl-2-pyrrolidinecarboxylic acid, M-60126
1-Nitro-3-hexene, N-70051
3-Piperidinecarboxylic acid, P-70102

$C_6H_{11}NO_3$
2-Amino-1-hydroxy-1-cyclobutaneacetic acid, A-60184
1-Amino-3-(hydroxymethyl)-1-cyclobutanecarboxylic acid, A-70157
1-Amino-3-(hydroxymethyl)cyclobutanecarboxylic acid, A-80082
2-Amino-2-(hydroxymethyl)-4-pentenoic acid, A-60190
Ethyl ethoxyiminoacetate, E-80063

$C_6H_{11}NO_4$
L-Allothreonine; *N*-Ac, *in* T-60217
2-Amino-3,3-dimethylbutanedioic acid, A-60147
2-Amino-3-ethylbutanedioic acid, A-70138
2-Amino-4-methylpentanedioic acid, A-60223

$C_6H_{11}NS_2$
5,6-Dihydro-2-(ethylthio)-4*H*-1,3-thiazine, *in* T-60094
Tetrahydro-2*H*-1,3-thiazine-2-thione; *N*-Et, *in* T-60094

$C_6H_{11}N_3O$
2-Azidocyclohexanol, A-80196

$C_6H_{11}N_3O_2$
Dihydro-1,3,5-triazine-2,4(1*H*,3*H*)-dione; 1,3,5-Tri-Me, *in* D-60297

$C_6H_{11}N_5$
2,4,6-Triaminopyrimidine; N^2,N^2-Di-Me, *in* T-80208
2,4,6-Triaminopyrimidine; N^4,N^4-Di-Me, *in* T-80208
2,4,6-Triaminopyrimidine; N^4-Et, *in* T-80208
2,4,6-Triaminopyrimidine; N^4,N^6-Di-Me, *in* T-80208

$C_6H_{11}O_9P$
myo-Inositol; 1-Phosphate, *in* I-80015

$C_6H_{12}BrCl$
1-Bromo-6-chlorohexane, B-70200

$C_6H_{12}BrN$
2-(Bromomethyl)cyclopentanamine, B-70240

$C_6H_{12}BrNO_2$
6-Amino-2-bromohexanoic acid, A-60100

$C_6H_{12}Br_2$
1,3-Dibromo-2,3-dimethylbutane, D-70089

$C_6H_{12}Br_2O_2$
1,6-Dibromo-3,4-hexanediol, D-80095

$C_6H_{12}ClNO_2$
6-Amino-2-chlorohexanoic acid, A-60109

$C_6H_{12}I_2O_2$
1,2-Bis(2-iodoethoxy)ethane, B-60163

$C_6H_{12}NO_2^{\oplus}$
4-Azoniaspiro[3.3]heptane-2,6-diol, A-60354

$C_6H_{12}N_2$
4-Cyclohexene-1,2-diamine, C-80180
▷ 1,4-Diazabicyclo[2.2.2]octane, D-70051
2-Dimethylamino-3,3-dimethylazirine, D-60402
1,3-Dimethyl-2-methyleneimidazolidine, D-70420
5-Hexyne-1,4-diamine, H-60080
Octahydropyrrolo[3,4-*c*]pyrrole, O-70017
Tetrahydro-1*H*,5*H*-pyrazolo[1,2-*a*]pyrazole, T-80077

$C_6H_{12}N_2O$
3-Amino-2-hexenoic acid; Amide, *in* A-60170
3-Piperidinecarboxamide, *in* P-70102
▷ 3,4,5,6-Tetrahydro-2(1*H*)-pyrimidinone, *in* T-60088

$C_6H_{12}N_2O_3$
3,3′-Oxybispropanoic acid; Diamide, *in* O-80098

$C_6H_{12}N_2O_3S$
N-Alanylcysteine, A-60069

$C_6H_{12}N_2O_4$
3,4,8,9-Tetraoxa-1,6-diazabicyclo[4.4.2]dodecane, T-70144

$C_6H_{12}N_4$
1,2,3,4,5,6,7,8-Octahydropyridazino[4,5-*d*]pyridazine, O-60018

$C_6H_{12}N_4O_2$
2,5-Piperazinedicarboxylic acid; Diamide, *in* P-60157

$C_6H_{12}N_6$
▷ Benzenehexamine, B-80014

$C_6H_{12}O$
2,3-Dimethyl-3-buten-1-ol, D-80439
2,2-Dimethylcyclopropanemethanol, D-70396
4-Hexen-3-ol, H-60077
1-Methoxy-2,3-dimethylcyclopropane, *in* D-70397
3-Methyl-2-pentanone, M-70105
▷ 4-Methyl-2-pentanone, M-60109
2-Methyl-4-penten-1-ol, M-80135
4-Methyl-1-penten-3-ol, M-70107
Tetrahydro-2-methylpyran, T-60075
Tetrahydro-3-methyl-2*H*-pyran, T-80072
Tetrahydro-4-methyl-2*H*-pyran, T-80073

$C_6H_{12}OS$
2-Mercaptocyclohexanol, M-70024
3,3,4,4-Tetramethyl-1,2-oxathietane, T-60149

$C_6H_{12}O_2$
β,*β*-Dimethyloxiraneethanol, D-60431

2-Hexene-1,6-diol, H-80081
3-Hexene-1,6-diol, H-80082
3-Hexene-2,5-diol, H-80083
2-(2-Propenyl)-1,3-propanediol, P-80180

$C_6H_{12}O_2S$
3-Mercaptobutanoic acid; Et ester, *in* M-70023
2-Mercapto-3-methylpentanoic acid, M-80026
2-Mercapto-4-methylpentanoic acid, M-80027

$C_6H_{12}O_2S_2$
2,5-Dimethyl-1,4-dithiane-2,5-diol, D-60421

$C_6H_{12}O_3$
▷ 2-Acetoxy-1-methoxypropane, *in* P-70118
Diethoxyacetaldehyde, D-70153
1,1-Dimethoxy-2-butanone, *in* O-80067
3-Hydroxy-2-methylpentanoic acid, H-80209
3-Hydroxy-3-methylpentanoic acid, H-80210
5-Hydroxy-3-methylpentanoic acid, H-70182

$C_6H_{12}O_3S$
Sulfoacetic acid; Di-Et ester, *in* S-80050

$C_6H_{12}O_4$
3,4-Dihydroxybutanoic acid; Et ester, *in* D-60313
5,6-Dihydroxyhexanoic acid, D-60329
2,5-Dihydroxy-3-methylpentanoic acid, D-60353
▷ Tetramethoxyethene, T-80135

$C_6H_{12}O_6$
myo-Inositol, I-80015

$C_6H_{12}S_2$
1,1-Cyclobutanedimethanethiol, C-70213
1,2-Cyclobutanedimethanethiol, C-70214
▷ 1,1-Cyclohexanedithiol, C-60209
1,2-Cyclohexanedithiol, C-70225
1,2-Dithiocane, D-50815

$C_6H_{13}Br$
1-Bromo-3-methylpentane, B-80223

$C_6H_{13}N$
2,5-Dimethylpyrrolidine, D-70437
4-Hexen-1-amine, H-70088
5-Hexen-1-amine, H-80078
2,2,3,3-Tetramethylaziridine, T-80139

$C_6H_{13}NO$
▷ *N*-Cyclohexylhydroxylamine, C-70228

$C_6H_{13}NO_2$
2-Amino-2,3-dimethylbutanoic acid, A-60148
2-Amino-3,3-dimethylbutanoic acid, A-70136

$C_6H_{13}NO_2S$
2-Amino-5-(methylthio)pentanoic acid, A-60231

$C_6H_{13}NO_3$
2-Amino-4-ethoxybutanoic acid, *in* A-70156

$C_6H_{13}NS$
2-[(Methylthio)methyl]pyrrolidine, *in* P-70185

$C_6H_{13}N_3O_2$
Biuret; 1,1,3,5-Tetra-Me, *in* B-60190

$C_6H_{13}N_3O_3$
Citrulline, C-60151

$C_6H_{14}ClN_3$
Gold's reagent; Chloride, *in* G-80032

$C_6H_{14}ClN_3O_4$
Gold's reagent; Perchlorate, *in* G-80032

$C_6H_{14}Cl_6N_3Sb$
Gold's reagent; Hexachloroantimonate, *in* G-80032

$C_6H_{14}N_2$
Hexahydropyrimidine; 1,3-Di-Me, *in* H-60056

$C_6H_{14}N_2O$
2-Amino-3,3-dimethylbutanoic acid; Amide, *in* A-70136

$C_6H_{14}N_2O_2$
3,4-Diaminohexanoic acid, D-80059
5,6-Diaminohexanoic acid, D-80060
2,5-Diamino-2-methylpentanoic acid, D-80061

$C_6H_{14}N_3^{\oplus}$
Gold's reagent, G-80032

$C_6H_{14}N_4O_3$
2-Amino-5-guanidino-3-hydroxypentanoic acid, A-70149

$C_6H_{14}O_2S$
2,2-Diethoxyethanethiol, *in* M-80017
2-(Ethylthio)-1,1-dimethoxyethane, *in* M-80017

$C_6H_{14}O_2S_2$
S,S'-Bis(2-hydroxyethyl)-1,2-ethanedithiol, B-70145

$C_6H_{14}O_3$
1,1-Dimethoxy-2-butanol, *in* H-70112
3,3'-Oxybis-1-propanol, O-60097

$C_6H_{14}O_4$
2,3-Bis(hydroxymethyl)-1,4-butanediol, B-60159

$C_6H_{14}O_6S_2$
S,S'-Bis(2-hydroxyethyl)-1,2-ethanedithiol; *S*-Tetroxide, *in* B-70145

$C_6H_{14}S_4$
S,S'-Bis(2-mercaptoethyl)-1,2-ethanedithiol, B-70150

$C_6H_{15}NO_2$
4,4-Dimethoxybutylamine, *in* A-80064

$C_6H_{15}N_3$
▷ Hexahydro-1,3,5-trimethyl-1,3,5-triazine, *in* H-60060

$C_6H_{15}O_{15}P_3$
myo-Inositol-1,3,4-triphosphate, I-70020
myo-Inositol-2,4,5-triphosphate, I-70021

$C_6H_{16}N_2O_2$
1,2-Bis(2-aminoethoxy)ethane, B-60139

$C_6H_{16}O_{18}P_4$
myo-Inositol-1,3,4,5-tetraphosphate, I-70019

$C_6H_{18}N_4$
1,2-Dihydrazinoethane; $N^{\beta},N^{\beta},N^{\beta'},N^{\beta'}$-Tetra-Me, *in* D-60192

$C_6H_{18}O_{24}P_6$
▷ Phytic acid, *in* I-80015

C_6N_4
▷ Tetracyanoethylene, T-60031

C_6N_4O
▷ Tetracyanooxirane, T-80023

C_6O_6
Cyclohexanehexone, C-60210

C_7F_5N
Pentafluoroisocyanobenzene, P-60036

C_7F_5NO
Pentafluoroisocyanatobenzene, P-60035

C_7F_5NS
Pentafluoroisothiocyanatobenzene, P-60037

C_7HF_4N
2,3,4,5-Tetrafluorobenzonitrile, *in* T-70032
2,3,5,6-Tetrafluorobenzonitrile, *in* T-70034

C_7HF_5
▷ Ethynylpentafluorobenzene, E-80075

$C_7HF_5O_2$
Pentafluorophenyl formate, P-70025

$C_7H_2BrF_5$
▷ (Bromomethyl)pentafluorobenzene, B-80222

$C_7H_2ClF_3N_2O_4$
▷ 2-Chloro-1,3-dinitro-5-(trifluoromethyl)benzene, C-80053

$C_7H_2ClF_5$
▷ (Chloromethyl)pentafluorobenzene, C-80072

$C_7H_2ClN_3O_7$
▷ 2,4,6-Trinitrobenzoic acid; Chloride, *in* T-70303

$C_7H_2F_3N$
2,4,5-Trifluorobenzonitrile, *in* T-70240

$C_7H_2F_4O$
2,3,4,5-Tetrafluorobenzaldehyde, T-70026
2,3,4,6-Tetrafluorobenzaldehyde, T-70027
2,3,5,6-Tetrafluorobenzaldehyde, T-70028

$C_7H_2F_4O_2$
2,3,4,5-Tetrafluorobenzoic acid, T-70032
2,3,4,6-Tetrafluorobenzoic acid, T-70033
2,3,5,6-Tetrafluorobenzoic acid, T-70034

$C_7H_3BrF_3NO_2$
1-Bromo-2-nitro-3-(trifluoromethyl)benzene, B-60306
1-Bromo-4-nitro-2-(trifluoromethyl)benzene, B-60307
2-Bromo-1-nitro-3-(trifluoromethyl)benzene, B-60308

$C_7H_3Br_4Cl$
1,2,4,5-Tetrabromo-3-chloro-6-methylbenzene, T-60022

$C_7H_3ClFNO_4$
2-Chloro-4-fluoro-5-nitrobenzoic acid, C-60072

$C_7H_3ClF_3NO_2$
4-Chloro-1-nitro-2-(trifluoromethyl)benzene, C-80086

$C_7H_3ClF_3N_3$
6-Chloro-2-(trifluoromethyl)-1*H*-imidazo[4,5-*b*]pyridine, C-60139

$C_7H_3ClF_3N_3O$
6-Chloro-2-(trifluoromethyl)-1*H*-imidazo[4,5-*b*]pyridine; 4-Oxide, *in* C-60139

$C_7H_3ClN_2O_5$
2,6-Dinitrobenzoic acid; Chloride, *in* D-60457
▷ 3,5-Dinitrobenzoic acid; Chloride, *in* D-60458

$C_7H_3Cl_3O$
2,3,4-Trichloro-2,4,6-cycloheptatrien-1-one, T-80224

$C_7H_3Cl_4N_3$
4,5,6,7-Tetrachlorobenzotriazole; 1-Me, *in* T-60027
4,5,6,7-Tetrachlorobenzotriazole; 2-Me, *in* T-60027

C_7H_3FIN
2-Cyano-1-fluoro-3-iodobenzene, *in* F-70020

$C_7H_3F_3N_2O_4$
1,3-Dinitro-5-(trifluoromethyl)benzene, D-70455
2,4-Dinitro-1-(trifluoromethyl)benzene, D-70456

$C_7H_3F_3O_2$
2,3,5-Trifluorobenzoic acid, T-70238
2,3,6-Trifluorobenzoic acid, T-70239
2,4,5-Trifluorobenzoic acid, T-70240

$C_7H_3F_5$
Pentafluoromethylbenzene, P-60038

$C_7H_3F_6N$
2,3-Bis(trifluoromethyl)pyridine, B-60181
2,4-Bis(trifluoromethyl)pyridine, B-60182
2,5-Bis(trifluoromethyl)pyridine, B-60183
2,6-Bis(trifluoromethyl)pyridine, B-60184
3,4-Bis(trifluoromethyl)pyridine, B-60185
3,5-Bis(trifluoromethyl)pyridine, B-60186

$C_7H_3F_6NO$
2,4-Bis(trifluoromethyl)pyridine; 1-Oxide, *in* B-60182
2,5-Bis(trifluoromethyl)pyridine; 1-Oxide, *in* B-60183
2,6-Bis(trifluoromethyl)pyridine; 1-Oxide, *in* B-60184

C_7H_3NS
▷ 2,4-Diethynylthiazole, D-80156

$C_7H_3N_3O_4$
▷ 1-Cyano-3,5-dinitrobenzene, *in* D-60458
2-Cyano-1,3-dinitrobenzene, *in* D-60457

$C_7H_3N_3O_8$
▷ 2,4,6-Trinitrobenzoic acid, T-70303

$C_7H_4BrFO_2$
2-Bromo-4-fluorobenzoic acid, B-60240
2-Bromo-5-fluorobenzoic acid, B-60241
2-Bromo-6-fluorobenzoic acid, B-60242
3-Bromo-4-fluorobenzoic acid, B-60243

C_7H_4BrN
5-Bromo-2-ethynylpyridine, B-80203

$C_7H_4BrNO_3$
4-Bromo-2-nitrobenzaldehyde, B-80235
4-Bromo-3-nitrobenzaldehyde, B-80236
▷ 5-Bromo-2-nitrobenzaldehyde, B-80237

C_7H_4ClFO
3-Chloro-4-fluorobenzaldehyde, C-70067

$C_7H_4ClF_3O_2S$
2-(Trifluoromethyl)benzenesulfonic acid; Chloride, *in* T-70242
▷ 3-(Trifluoromethyl)benzenesulfonic acid; Chloride, *in* T-60283
4-(Trifluoromethyl)benzenesulfonic acid; Chloride, *in* T-70243

C_7H_4ClNO
▷ 2-Chlorobenzoxazole, C-60048
2-Chloro-4-cyanophenol, *in* C-60091

C_7H_4ClNS
4-Chloro-1,2-benzisothiazole, C-70050
5-Chloro-1,2-benzisothiazole, C-70051
6-Chloro-1,2-benzisothiazole, C-70052
7-Chloro-1,2-benzisothiazole, C-70053
2-Chloro-6-cyanobenzenethiol, *in* C-70083

$C_7H_4Cl_2O_2$
2,2-Dichloro-1,3-benzodioxole, D-70113
2,5-Dichloro-4-hydroxybenzaldehyde, D-70120
2,6-Dichloro-4-hydroxybenzaldehyde, D-70121

$C_7H_4Cl_2O_3$
2,3-Dichloro-4-hydroxybenzoic acid, D-60133

$C_7H_4FIO_2$
2-Fluoro-6-iodobenzoic acid, F-70020
3-Fluoro-2-iodobenzoic acid, F-70021
3-Fluoro-4-iodobenzoic acid, F-70022
4-Fluoro-2-iodobenzoic acid, F-70023
4-Fluoro-3-iodobenzoic acid, F-70024
5-Fluoro-2-iodobenzoic acid, F-70025

C_7H_4FNO
▷ 1-Fluoro-2-isocyanatobenzene, F-60047
▷ 1-Fluoro-3-isocyanatobenzene, F-60048
▷ 1-Fluoro-4-isocyanatobenzene, F-60049

$C_7H_4FNO_4$
3-Fluoro-4-nitrobenzoic acid, F-70033

C_7H_4FNS
4-Cyano-3-fluorobenzenethiol, *in* F-70029
1-Fluoro-4-isothiocyanatobenzene, F-80049

$C_7H_4F_2$
7,7-Difluorobicyclo[4.1.0]hepta-1,3,5-triene, D-60177

$C_7H_4F_3NO_2$
▷ 1-Nitro-2-(trifluoromethyl)benzene, N-70064
▷ 1-Nitro-3-(trifluoromethyl)benzene, N-70065
▷ 1-Nitro-4-(trifluoromethyl)benzene, N-70066

$C_7H_4F_3NO_3$
2-Nitro-3-(trifluoromethyl)phenol, N-60047
▷ 2-Nitro-4-(trifluoromethyl)phenol, N-60048
2-Nitro-5-(trifluoromethyl)phenol, N-60049
2-Nitro-6-(trifluoromethyl)phenol, N-60050
3-Nitro-4-(trifluoromethyl)phenol, N-60051
3-Nitro-5-(trifluoromethyl)phenol, N-60052
4-Nitro-2-(trifluoromethyl)phenol, N-60053
▷ 4-Nitro-3-(trifluoromethyl)phenol, N-60054

$C_7H_4INO_3$
2-Iodo-6-nitrobenzaldehyde, I-80038
5-Iodo-2-nitrobenzaldehyde, I-60052

$C_7H_4I_2O_2$
2,3-Diiodobenzoic acid, D-80396

$C_7H_4N_2O_2S$
5-Nitro-1,2-benzisothiazole, N-70041
7-Nitro-1,2-benzisothiazole, N-70042

$C_7H_4N_2O_3$
6-Diazo-5-oxo-1,3-cyclohexadiene-1-carboxylic acid, D-70063

$C_7H_4N_2O_6$
2,6-Dinitrobenzoic acid, D-60457
3,5-Dinitrobenzoic acid, D-60458

$C_7H_4N_4$
2-Amino-3,5-dicyanopyridine, *in* A-70193

$C_7H_4N_4O_7$
2,4,6-Trinitrobenzoic acid; Amide, *in* T-70303

$C_7H_4N_6O_6$
3,5-Diamino-2,4,6-trinitrobenzoic acid; Nitrile, *in* D-70047

C_7H_4O
2,6-Cycloheptadien-4-yn-1-one, C-60196

C_7H_4OS
Benzothiet-2-one, B-70065

C_7H_4OSSe
1,3-Benzoxathiole-2-selone, B-70070

$C_7H_4O_2$
Bicyclo[4.1.0]hepta-1(6),3-diene-2,5-dione, B-80078

$C_7H_4O_2S$
1,3-Benzodioxole-2-thione, B-80022
3-(2-Thienyl)-2-propynoic acid, T-70173

$C_7H_4O_3S$
4*H*-Thieno[3,4-*c*]pyran-4,6(7*H*)-dione, *in* C-60018
5*H*-Thieno[2,3-*c*]pyran-5,7(4*H*)dione, *in* C-60017

$C_7H_4O_4$
1,2-Benzoquinone-3-carboxylic acid, B-70045
1,2-Benzoquinone-4-carboxylic acid, B-70046

$C_7H_4O_5$
3-Oxotricyclo[2.1.0.0^{2,5}]pentane-1,5-dicarboxylic acid, O-80096

$C_7H_4SSe_2$
1,3-Benzodiselenole-2-thione, B-70032

$C_7H_4S_2Se$
3*H*-1,2-Benzodithiole-3-selone, B-70034

C_7H_5Br
2-Bromobenzocyclopropene, B-60202
3-Bromobenzocyclopropene, B-60203

$C_7H_5BrCl_2O$
1-Bromo-2,3-dichloro-4-methoxybenzene, *in* B-60229

$C_7H_5BrN_2O_3$
4-Bromo-2-nitrobenzaldehyde; Oxime, *in* B-80235
4-Bromo-3-nitrobenzaldehyde; Oxime, *in* B-80236
5-Bromo-2-nitrobenzaldehyde; Oxime, *in* B-80237

$C_7H_5BrN_4$
5-Bromo-1*H*-tetrazole; 1-Ph, *in* B-80262

$C_7H_5BrO_2S$
2-Bromo-4-mercaptobenzoic acid, B-70226
2-Bromo-5-mercaptobenzoic acid, B-70227
3-Bromo-4-mercaptobenzoic acid, B-70228

$C_7H_5Br_3OS$
[(Tribromomethyl)sulfinyl]benzene, *in* T-70212

$C_7H_5Br_3O_2S$
[(Tribromomethyl)sulfonyl]benzene, *in* T-70212

$C_7H_5Br_3S$
[(Tribromomethyl)thio]benzene, T-70212

$C_7H_5Br_4N$
2,3-Bis(dibromomethyl)pyridine, B-60151
3,4-Bis(dibromomethyl)pyridine, B-60152

$C_7H_5ClN_4$
5-Chlorotetrazole; 1-Ph, *in* C-80113

C_7H_5ClOS
Carbonochloridothioic acid; *S*-Ph, *in* C-60013

$C_7H_5ClO_2$
3-Chloro-4-hydroxybenzaldehyde, C-60089
4-Chloro-3-hydroxybenzaldehyde, C-60090
2-Hydroxybenzoic acid; Chloride, *in* H-70108

$C_7H_5ClO_2S$
2-Chloro-6-mercaptobenzoic acid, C-70082
3-Chloro-2-mercaptobenzoic acid, C-70083
4-Chloro-2-mercaptobenzoic acid, C-70084
5-Chloro-2-mercaptobenzoic acid, C-70085

$C_7H_5ClO_3$
2-Chloro-3,6-dihydroxybenzaldehyde, C-60056
3-Chloro-2,5-dihydroxybenzaldehyde, C-60057
3-Chloro-2,6-dihydroxybenzaldehyde, C-60058
5-Chloro-2,3-dihydroxybenzaldehyde, C-70065
3-Chloro-4-hydroxybenzoic acid, C-60091
3-Chloro-5-hydroxybenzoic acid, C-60092
4-Chloro-3-hydroxybenzoic acid, C-60093

$C_7H_5Cl_2NO_3$
2,3-Dichloro-1-methoxy-4-nitrobenzene, *in* D-70125

$C_7H_5FN_2$
2-Cyano-3-fluoroaniline, *in* A-70143
3-Cyano-4-fluoroaniline, *in* A-70147
4-Cyano-2-fluoroaniline, *in* A-70146
▷ 3-Fluoro-3-phenyl-3*H*-diazirine, F-70036

$C_7H_5FN_2O_4$
5-Fluoro-2-methyl-1,3-dinitrobenzene, F-60051

$C_7H_5FO_2$
2-Fluoro-3-hydroxybenzaldehyde, F-60035
2-Fluoro-5-hydroxybenzaldehyde, F-60036
4-Fluoro-3-hydroxybenzaldehyde, F-60037

$C_7H_5FO_2S$
2-Fluoro-4-mercaptobenzoic acid, F-70029
2-Fluoro-6-mercaptobenzoic acid, F-70030
4-Fluoro-2-mercaptobenzoic acid, F-70031

$C_7H_5FO_3$
2-Fluoro-5-hydroxybenzoic acid, F-60038
2-Fluoro-6-hydroxybenzoic acid, F-60039
3-Fluoro-2-hydroxybenzoic acid, F-60040
3-Fluoro-4-hydroxybenzoic acid, F-60041
4-Fluoro-2-hydroxybenzoic acid, F-60042
4-Fluoro-3-hydroxybenzoic acid, F-60043
5-Fluoro-2-hydroxybenzoic acid, F-60044

$C_7H_5FO_4$
3-Fluoro-2,6-dihydroxybenzoic acid, F-60023
4-Fluoro-3,5-dihydroxybenzoic acid, F-60024
5-Fluoro-2,3-dihydroxybenzoic acid, F-60025

$C_7H_5F_3O_3S$
2-(Trifluoromethyl)benzenesulfonic acid, T-70242
3-(Trifluoromethyl)benzenesulfonic acid, T-60283
4-(Trifluoromethyl)benzenesulfonic acid, T-70243

$C_7H_5F_3S$
2-(Trifluoromethyl)benzenethiol, T-60284
3-(Trifluoromethyl)benzenethiol, T-60285
4-(Trifluoromethyl)benzenethiol, T-60286

$C_7H_5IN_4$
5-Iodo-1*H*-tetrazole; 1-Ph, *in* I-80042

$C_7H_5IO_2$
2-Hydroxy-5-iodobenzaldehyde, H-70143

$C_7H_5IO_2S$
3-Iodo-4-mercaptobenzoic acid, I-70046

$C_7H_5IO_3$
▷ 1-Hydroxy-1,2-benziodoxol-3(1*H*)-one, H-60102

$C_7H_5IO_4$
2,3-Dihydroxy-6-iodobenzoic acid, D-60330
2,4-Dihydroxy-3-iodobenzoic acid, D-60331
2,4-Dihydroxy-5-iodobenzoic acid, D-60332
2,5-Dihydroxy-4-iodobenzoic acid, D-60333

2,6-Dihydroxy-3-iodobenzoic acid, D-60334
3,4-Dihydroxy-5-iodobenzoic acid, D-60335
3,5-Dihydroxy-2-iodobenzoic acid, D-60336
3,5-Dihydroxy-4-iodobenzoic acid, D-60337
4,5-Dihydroxy-2-iodobenzoic acid, D-60338

$C_7H_5I_2O_2$
2,6-Diiodobenzoic acid, D-70356

C_7H_5N
2-Ethynylpyridine, E-80076
3-Ethynylpyridine, E-80077
4-Ethynylpyridine, E-80078

C_7H_5NO
Benzonitrile *N*-oxide, B-60035
2-Cyanophenol, *in* H-70108
4-Ethynylpyridine; N-Oxide, *in* E-80078
3-Ethynylpyridine; *N*-oxide, *in* E-80077

C_7H_5NOS
5-(2-Thienyl)oxazole, T-70171

$C_7H_5NO_2$
5-(2-Furanyl)oxazole, F-70048
4-Nitrosobenzaldehyde, N-60046

$C_7H_5NO_2S$
1,2,3-Benzoxathiazin-4(3*H*)-one, B-80052

$C_7H_5NO_3$
4-Hydroxy-3-nitrosobenzaldehyde, H-60197

$C_7H_5NO_4$
4-Hydroxy-3-nitrosobenzoic acid, H-70193

$C_7H_5NO_4S$
1,2,3-Benzoxathiazin-4(3*H*)-one; 2,2-Dioxide, *in* B-80052

$C_7H_5NO_6$
4,5-Dihydroxy-2-nitrobenzoic acid, D-60360

$C_7H_5NS_2$
Benzenesulfenyl thiocyanate, B-60013

C_7H_5NSe
Benzoselenazole, B-70050

$C_7H_5N_3OS$
2,3-Dihydro-2-thioxopyrido[2,3-*d*]pyrimidin-4(1*H*)-one, D-60291
2,3-Dihydro-2-thioxopyrido[3,2-*d*]pyrimidin-4(1*H*)-one, D-60292
2,3-Dihydro-2-thioxopyrido[3,4-*d*]pyrimidin-4(1*H*)-one, D-60293
2,3-Dihydro-2-thioxo-4*H*-pyrido[1,2-*a*]-1,3,5-triazin-4-one, D-60294

$C_7H_5N_3O_2$
Pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione, P-60236
Pyrido[3,4-*d*]pyrimidine-2,4(1*H*,3*H*)-dione, P-60237

$C_7H_5N_3O_2S$
3-Amino-5-nitro-2,1-benzisothiazole, A-60232

$C_7H_5N_3O_5$
3,5-Dinitrobenzamide, *in* D-60458

$C_7H_5N_3S$
1,2,3-Benzotriazine-4(3*H*)-thione, B-60050
2-(1,3,4-Thiadiazol-2-yl)pyridine, T-60192
4-(1,3,4-Thiadiazol-2-yl)pyridine, T-60193

$C_7H_5N_5O$
1*H*-Imidazo[2,1-*b*]purin-4(5*H*)-one, I-70006

$C_7H_5N_5O_3$
2-Amino-4(3*H*)-pteridinone-6-carboxylic acid, A-80135

$C_7H_5N_5O_8$
3,5-Diamino-2,4,6-trinitrobenzoic acid, D-70047
▷ 2-Methyl-3,4,5,6-tetranitroaniline, M-60129
▷ 3-Methyl-2,4,5,6-tetranitroaniline, M-60130
▷ 4-Methyl-2,3,5,6-tetranitroaniline, M-60131
2,3,4,6-Tetranitroaniline; *N*-Me, *in* T-60159

C_7H_6
1*H*-Cyclopropabenzene, C-70246

C_7H_6BrF
▷ 1-(Bromomethyl)-2-fluorobenzene, B-80215
▷ 1-(Bromomethyl)-3-fluorobenzene, B-80216
▷ 1-(Bromomethyl)-4-fluorobenzene, B-80217

C_7H_6BrFO
3-Bromo-4-fluorobenzyl alcohol, B-60244
5-Bromo-2-fluorobenzyl alcohol, B-60245
2-Bromo-1-fluoro-3-methoxybenzene, *in* B-60247
2-Bromo-4-fluoro-1-methoxybenzene, *in* B-60248
4-Bromo-2-fluoro-1-methoxybenzene, *in* B-60251

$C_7H_6BrNO_2$
3-Amino-2-bromobenzoic acid, A-70097

$C_7H_6BrNO_3$
2-Bromo-1-methoxy-3-nitrobenzene, *in* B-70257
2-Bromo-3-nitrobenzyl alcohol, B-70256
4-Bromo-2-nitrobenzyl alcohol, B-80238

$C_7H_6Br_2$
1,3-Dibromo-2-methylbenzene, D-60103

C_7H_6ClFO
1-Chloro-2-fluoro-4-methoxybenzene, *in* C-60080
1-Chloro-4-fluoro-2-methoxybenzene, *in* C-60074
2-Chloro-4-fluoro-1-methoxybenzene, *in* C-60073
4-Chloro-2-fluoro-1-methoxybenzene, *in* C-60079

C_7H_6ClNO
2-Acetyl-5-chloropyridine, A-70033
3-Acetyl-2-chloropyridine, A-70034
4-Acetyl-2-chloropyridine, A-70035
4-Acetyl-3-chloropyridine, A-70036
5-Acetyl-2-chloropyridine, A-70037

$C_7H_6ClNO_2$
3-Chloro-4-hydroxybenzoic acid; Amide, *in* C-60091

$C_7H_6ClNO_3$
4-Chloro-2-methoxy-1-nitrobenzene, *in* C-60119
2-Chloro-3-methyl-4-nitrophenol, C-60115
3-Chloro-4-methyl-5-nitrophenol, C-60116

$C_7H_6Cl_2O_2$
Bicyclo[1.1.1]pentane-1,3-dicarboxylic acid; Dichloride, *in* B-80090

$C_7H_6Cl_2S$
1,2-Dichloro-4-(methylthio)benzene, *in* D-60123
1,4-Dichloro-2-(methylthio)benzene, *in* D-60121

$C_7H_6FNO_2$
2-Amino-3-fluorobenzoic acid, A-70140
2-Amino-4-fluorobenzoic acid, A-70141
2-Amino-5-fluorobenzoic acid, A-70142
2-Amino-6-fluorobenzoic acid, A-70143
3-Amino-4-fluorobenzoic acid, A-70144
4-Amino-2-fluorobenzoic acid, A-70145
▷ 4-Amino-3-fluorobenzoic acid, A-70146
5-Amino-2-fluorobenzoic acid, A-70147
4-Fluoro-2-hydroxybenzoic acid; Amide, *in* F-60042

$C_7H_6FNO_3$
4-Fluoro-2-methoxy-1-nitrobenzene, *in* F-60061

$C_7H_6F_2S$
1,3-Difluoro-2-(methylthio)benzene, *in* D-60174
1,3-Difluoro-5-(methylthio)benzene, *in* D-60176
1,4-Difluoro-2-(methylthio)benzene, *in* D-60173

$C_7H_6F_3NO_2$
2-Hydroxy-3-methyl-2-butenenitrile; Trifluoroacetyl, *in* H-80198

$C_7H_6F_3NO_2S$
2-(Trifluoromethyl)benzenesulfonic acid; Amide, *in* T-70242
3-(Trifluoromethyl)benzenesulfonic acid; Amide, *in* T-60283
4-(Trifluoromethyl)benzenesulfonic acid; Amide, *in* T-70243

$C_7H_6INO_2$
2-Hydroxy-5-iodobenzaldehyde; Oxime, *in* H-70143

$C_7H_6N_2$
3-Phenyl-3*H*-diazirine, P-70067
Pyrrolo[1,2-*a*]pyrazine, P-70197
▷ 1*H*-Pyrrolo[3,2-*b*]pyridine, P-60249
6*H*-Pyrrolo[3,4-*b*]pyridine, P-70201
2*H*-Pyrrolo[3,4-*c*]pyridine, P-70200

$C_7H_6N_2O$
▷ 2-Aminobenzoxazole, A-60093
1,6-Dihydro-7*H*-pyrrolo[2,3-*c*]pyridin-7-one, D-80252
Pyrrolo[1,2-*a*]pyrazin-1(2*H*)-one, P-70198

$C_7H_6N_2O_3S$
1*H*-Benzimidazole-2-sulfonic acid, B-70022

$C_7H_6N_2O_4$
2-Amino-3,5-pyridinedicarboxylic acid, A-70193
4-Amino-2,6-pyridinedicarboxylic acid, A-70194
5-Amino-3,4-pyridinedicarboxylic acid, A-70195
▷ Antibiotic 2061 *A*, *in* A-70158
▷ 2-Methyl-1,3-dinitrobenzene, M-60061

$C_7H_6N_2O_5$
2,6-Dinitrobenzyl alcohol, D-60459

$C_7H_6N_2O_6$
2-Methoxy-4,5-dinitrophenol, *in* D-70449
5-Methoxy-2,4-dinitrophenol, *in* D-80491

$C_7H_6N_4$
4-Amino-1,2,3-benzotriazine, A-60092
2-Methylpteridine, M-70120
4-Methylpteridine, M-70121
6-Methylpteridine, M-70122
7-Methylpteridine, M-70123

$C_7H_6N_4O$
4-Amino-1,2,3-benzotriazine; 2-Oxide, *in* A-60092
4-Amino-1,2,3-benzotriazine; 3-Oxide, *in* A-60092
2-Amino-5-cyanonicotinamide, *in* A-70193
Di-1*H*-imidazol-2-ylmethanone, D-70354
4-Hydroxylamino-1,2,3-benzotriazine, *in* A-60092

$C_7H_6N_4O_2$
2,4(1*H*,3*H*)-Pteridinedione; 1-Me, *in* P-60191
2,4(1*H*,3*H*)-Pteridinedione; 3-Me, *in* P-60191

$C_7H_6N_4O_3$
6-(Hydroxymethyl)-2,4(1*H*,3*H*)pteridinedione, H-80213
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione; I-Me, *in* P-70134
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione; 3-Me, *in* P-70134
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione; 7-Me, *in* P-70134
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 3-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 6-Me, *in* P-70135

$C_7H_6N_4O_6$
2,4,6-Trinitroaniline; *N*-Me, *in* T-70301

$C_7H_6N_4S$
1*H*-Tetrazole-5-thiol; *S*-Ph, *in* T-60174
▷ Tetrazole-5-thione; 1-Ph, *in* T-60174

C_7H_6O
2,4,6-Cycloheptatrien-1-one, C-60204
Dimethylenebicyclo[1.1.1]pentanone, D-60422

4-Methylene-2,5-cyclohexadien-1-one, M-60071
6-Methylene-2,4-cyclohexadien-1-one, M-60072

C_7H_6OS
4*H*-Cyclopenta[*c*]thiophen-5(6*H*)-one, C-70245
4,5-Dihydro-6*H*-cyclopenta[*b*]thiophen-6-one, D-70182
4,6-Dihydro-5*H*-cyclopenta[*b*]thiophen-5-one, D-70183
5,6-Dihydro-4*H*-cyclopenta[*c*]thiophen-4-one, D-70184
2-Mercaptobenzaldehyde, M-80018
3-Mercaptobenzaldehyde, M-80019
4-Mercaptobenzaldehyde, M-80020
3-(2-Thienyl)-2-propenal, T-80184
3-(3-Thienyl)-2-propenal, T-80185

$C_7H_6OS_2$
2,3-Dihydro-4*H*-thieno[2,3-*b*]thiopyran-4-one, D-80259
5,6-Dihydro-7*H*-thieno[3,2-*b*]thiopyran-7-one, D-80260
4*H*-Thieno[3,2-*c*]thiopyran-7(6*H*)-one, T-80177

$C_7H_6O_2$
Bicyclo[3.2.0]hept-2-ene-6,7-dione, B-70099

$C_7H_6O_2S$
3-(2-Thienyl)-2-propenoic acid, T-60208
3-(3-Thienyl)-2-propenoic acid, T-70172

$C_7H_6O_3$
2,3-Dihydroxybenzaldehyde, D-70285
2,3-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-80307
2,4-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-80308
2,5-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-80309
2,7-Dihydroxy-2,4,6-cycloheptatrien-1-one, D-60314
▷ 2-Hydroxybenzoic acid, H-70108

$C_7H_6O_4$
▷ 2,3-Dihydroxy-5-methyl-1,4-benzoquinone, D-70320
3-(Hydroxymethyl)-7-oxabicyclo[4.1.0]hept-3-ene-2,5-dione, H-70181

$C_7H_6O_4S$
2-Carboxy-3-thiopheneacetic acid, C-60017
4-Carboxy-3-thiopheneacetic acid, C-60018
2*H*-Thiopyran-2,2-dicarboxylic acid, T-80191

$C_7H_6O_5$
2,3,5-Trihydroxybenzoic acid, T-70250

$C_7H_6O_6$
Osbeckic acid, O-70048
Pentahydroxybenzaldehyde, P-60042
2,3,5,6-Tetrahydroxybenzoic acid, T-60100

$C_7H_6O_7$
Pentahydroxybenzoic acid, P-60043

C_7H_6S
2,4,6-Cycloheptatriene-1-thione, C-60203

$C_7H_6Se_2$
1,3-Benzodiselenole, B-70031

$C_7H_7BrO_3$
4-Bromo-2,6-dimethoxyphenol, *in* B-60201

C_7H_7BrSe
Bromomethyl phenyl selenide, B-60300

$C_7H_7Br_2N$
▷ 2,6-Bis(bromomethyl)pyridine, B-60146
3,5-Bis(bromomethyl)pyridine, B-60147

C_7H_7Cl
2-Chlorobicyclo[2.2.1]hepta-2,5-diene, C-70056

$C_7H_7ClN_2O_2$
2-Chloro-6-nitrobenzylamine, C-70126
4-Chloro-2-nitrobenzylamine, C-70127
4-Chloro-3-nitrobenzylamine, C-70128
5-Chloro-2-nitrobenzylamine, C-70129

C_7H_7ClO
2-(Chloromethyl)phenol, C-70101
3-(Chloromethyl)phenol, C-70102
4-(Chloromethyl)phenol, C-70103

$C_7H_7Cl_2N$
2,4-Bis(chloromethyl)pyridine, B-80143

$C_7H_7Cl_3O_2$
3,4-Dihydro-5-(trichloroacetyl)-2*H*-pyran, D-70272

C_7H_7FO
2-Fluoro-3-methylphenol, F-60052
2-Fluoro-4-methylphenol, F-60053
2-Fluoro-5-methylphenol, F-60054
2-Fluoro-6-methylphenol, F-60055
3-Fluoro-2-methylphenol, F-60056
3-Fluoro-4-methylphenol, F-60057
4-Fluoro-2-methylphenol, F-60058
4-Fluoro-3-methylphenol, F-60059
5-Fluoro-2-methylphenol, F-60060

$C_7H_7F_3O_2$
3,4-Dihydro-5-(trifluoroacetyl)-2*H*-pyran, D-70275

$C_7H_7IN_2O$
3-Amino-5-iodopyridine; N-Ac, *in* A-80092

C_7H_7IO
4-Iodo-3-methylphenol, I-60050

C_7H_7NO
2,3-Dihydrofuro[2,3-*b*]pyridine, D-70211
2,3-Dihydro-1*H*-pyrrolizin-1-one, D-60277
5-Methyl-3-pyridinecarboxaldehyde, M-80152
3-(1*H*-Pyrrol-2-yl)-2-propenal, P-70202

C_7H_7NOS
2,3-Dihydrothieno[2,3-*b*]pyridine; 1-Oxide, *in* D-70269

$C_7H_7NOS_2$
2,3-Dihydro-4*H*-thieno[2,3-*b*]thiopyran-4-one; Oxime, *in* D-80259
5,6-Dihydro-7*H*-thieno[3,2-*b*]thiopyran-7-one; Oxime, *in* D-80260
4*H*-Thieno[3,2-*c*]thiopyran-7(6*H*)-one; Oxime, *in* T-80177

$C_7H_7NO_2$
2-(Hydroxyacetyl)pyridine, H-70101
3-(Hydroxyacetyl)pyridine, H-70102
▷ 2-Hydroxybenzamide, *in* H-70108
(Nitromethyl)benzene, N-70053

$C_7H_7NO_2S$
(Phenylthio)nitromethane, P-60137
2(1*H*)-Pyridinethione; 1-Acetoxy, *in* P-60224

$C_7H_7NO_3$
1,4-Dihydro-6-methyl-4-oxo-3-pyridinecarboxylic acid, D-80224
1,6-Dihydro-3-methyl-6-oxo-2-pyridinecarboxylic acid, D-80225
1,6-Dihydro-5-methyl-6-oxo-2-pyridinecarboxylic acid, D-80226
2-Formyl-1*H*-pyrrole-3-carboxylic acid; Me ester, *in* F-80077
5-Formyl-1*H*-pyrrole-2-carboxylic acid; Me ester, *in* F-80079
3-Hydroxy-2(1*H*)-pyridinone; 3-Ac, *in* H-60223
5-Hydroxy-2(1*H*)-pyridinone; 5-Ac, *in* H-60225

$C_7H_7NO_3S$
4-Carboxy-3-thiopheneacetic acid; Acetamide, *in* C-60018

$C_7H_7NO_4$
2-Methyl-4-nitro-1,3-benzenediol, M-70097
1*H*-Pyrrole-3,4-dicarboxylic acid; Me ester, *in* P-70183

$C_7H_7NO_4S$
(Nitromethyl)sulfonylbenzene, *in* P-60137

C_7H_7NS
2,3-Dihydrothieno[2,3-*b*]pyridine, D-70269

$C_7H_7N_3$
▷ 7-Azidobicyclo[2.2.1]hepta-2,5-diene, A-70285
5*H*-Pyrrolo[2,3-*b*]pyrazine; 5-Me, *in* P-60248

$C_7H_7N_3O$
1,3-Dihydro-2*H*-imidazo[4,5-*c*]pyridin-2-one; 1-Me, *in* D-60250

$C_7H_7N_3S$
2-Hydrazinobenzothiazole, H-70095

$C_7H_7N_5O$
2-Amino-1-methyl-4(1*H*)-pteridinone, *in* A-60242
2-(Methylamino)-4(1*H*)-pteridinone, *in* A-60242

C_7H_8
Bicyclo[3.2.0]hepta-2,6-diene, B-70097
3-Buten-1-ynylcyclopropane, B-70293
1-Ethynylcyclopentene, E-70052
1,5-Heptadiyne, H-80025
4-Methylenebicyclo[3.1.0]hex-2-ene, M-60069
4-Methylene-1,2,5-hexatriene, M-70071
Tetracyclo[3.2.0.0^{1,6}.0^{2,6}]heptane, T-80024

$C_7H_8BrF_3NO_2$
4-Bromo-1-nitro-2-(trifluoromethyl)benzene, B-60309

C_7H_8BrN
2-(2-Bromoethyl)pyridine, B-70210
3-(2-Bromoethyl)pyridine, B-70211
2-Bromo-3-methylaniline, B-70234

C_7H_8BrNO
2-Bromo-3-ethoxypyridine, *in* B-60275
2-Bromo-3-methoxyaniline, *in* A-70099
2-Bromo-3-methoxy-6-methylpyridine, *in* B-60267

C_7H_8ClN
2-(Chloromethyl)-3-methylpyridine, C-70093
▷ 2-(Chloromethyl)-4-methylpyridine, C-70094
2-(Chloromethyl)-5-methylpyridine, C-70095
▷ 2-(Chloromethyl)-6-methylpyridine, C-70096
3-(Chloromethyl)-2-methylpyridine, C-70097
3-(Chloromethyl)-4-methylpyridine, C-70098
▷ 4-(Chloromethyl)-2-methylpyridine, C-70099
5-(Chloromethyl)-2-methylpyridine, C-70100

$C_7H_8ClNO_2$
2-Chloro-4,6-dimethoxypyridine, *in* C-70074
4-Chloro-2,6-dimethoxypyridine, *in* C-70073
4-Chloro-6-methoxy-1-methyl-2(1*H*)-pyridinone, *in* C-70073

$C_7H_8ClNO_2S$
N-Chloro-4-methylbenzenesulfonamide, C-80071

$C_7H_8N_2$
2,3-Dihydroimidazo[1,2-*a*]pyridine, D-70216
2,3-Dihydro-1*H*-pyrrolo[2,3-*b*]pyridine, D-70263
2,3-Dihydro-1*H*-pyrrolo[3,2-*c*] pyridine, D-80251
N-Phenylformamidine, P-60101

$C_7H_8N_2O$
2-Acetyl-3-aminopyridine, A-70022
2-Acetyl-5-aminopyridine, A-70023
3-Acetyl-2-aminopyridine, A-70024
3-Acetyl-4-aminopyridine, A-70025
4-Acetyl-2-aminopyridine, A-70026
4-Acetyl-3-aminopyridine, A-70027
5-Acetyl-2-aminopyridine, A-70028
2-(Aminoacetyl)pyridine, A-70085
3-(Aminoacetyl)pyridine, A-70086
4-(Aminoacetyl)pyridine, A-70087
2,3-Dihydro-1*H*-pyrrolo[2,3-*b*]pyridine; 7-Oxide, *in* D-70263
5-Methyl-3-pyridinecarboxaldehyde; Oxime, *in* M-80152
4-Oxoheptanedinitrile, *in* O-60071

$C_7H_8N_2OS$
5-Amino-2(1*H*)-pyridinethione; *N*-Ac, *in* A-80141

$C_7H_8N_2O_2$
5-Acetyl-2-aminopyridine; *N*-Oxide, *in* A-70028
1-Amino-2(1*H*)-pyridinone; *N*-Ac, *in* A-60248
2,4-Diaminobenzoic acid, D-60032
1,2-Diamino-4,5-methylenedioxybenzene, D-60038

1,3-Diisocyanatocyclopentane, D-60390
1-Methoxy-2-phenyldiazene 2-oxide, *in* H-70208
Urocanic acid; Me ester, *in* U-70005

$C_7H_8N_2O_3$
3-Amino-4-methyl-5-nitrophenol, A-60222
2-Amino-3-nitrobenzyl alcohol, A-80125
2-Amino-6-nitrobenzyl alcohol, A-80126
3-Amino-2-nitrobenzyl alcohol, A-80127
3-Amino-4-nitrobenzyl alcohol, A-80128
3-Amino-5-nitrobenzyl alcohol, A-60233
4-Ethoxy-2-nitropyridine, *in* N-70063

$C_7H_8N_2O_3S$
Aminoiminomethanesulfonic acid; *N*-Ph, *in* A-60210

$C_7H_8N_2O_4$
4-Amino-5-hydroxy-2-oxo-7-oxabicyclo[4.1.0]hept-3-ene-3-carboxamide, A-70158
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidineacetic acid; Me ester, *in* T-70060

$C_7H_8N_2O_5$
3-Amino-2(1*H*)-pyridinethione; N^3-Ac, *in* A-60247

$C_7H_8N_2Se$
Selenourea; *N*-Ph, *in* S-70031

$C_7H_8N_4$
1′-Methyl-1,5′-bi-1*H*-pyrazole, *in* B-60119
2,2′-Methylenebis-1*H*-imidazole, M-70064

$C_7H_8N_4O$
N-(4-Cyano-1-methyl-1*H*-pyrazol-5-yl)acetamide, *in* A-70192
1,3-Dihydro-1,3-dimethyl-2*H*-imidazo[4,5-*b*]pyrazin-2-one, *in* I-60006
1,4-Dihydro-1,4-dimethyl-2*H*-imidazo[4,5-*b*]pyrazin-2-one, *in* I-60006
2-Methoxy-4-methyl-4*H*-imidazo[4,5-*b*]pyrazine, *in* I-60006

$C_7H_8N_4O_2$
2-Amino-3,5-pyridinedicarboxylic acid; Diamide, *in* A-70193
1*H*-Pyrazolo[3,4-*d*]pyrimidine-4,6(5*H*,7*H*)-dione; 1,5-Di-Me, *in* P-60202
1*H*-Pyrazolo[3,4-*d*]pyrimidine-4,6(5*H*,7*H*)-dione; 5,7-Di-Me, *in* P-60202

$C_7H_8N_4S$
1,3-Dihydro-1,3-dimethyl-2*H*-imidazo[4,5-*b*]pyrazine-2-thione, *in* D-60247
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazine-6-thione; N^1,*S*-Di-Me, *in* D-70215
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazine-6-thione; N^2,*S*-Di-Me, *in* D-70215
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazine-6-thione; N^5,*S*-Di-Me, *in* D-70215
1,5-Dihydro-6*H*-imidazo[4,5-*c*]pyridazine-6-thione; N^7,*S*-Di-Me, *in* D-70215
1,7-Dihydro-6*H*-purine-6-thione; 1,9-Di-Me, *in* D-60270
1,7-Dihydro-6*H*-purine-6-thione; 3,7-Di-Me, *in* D-60270
1,7-Dihydro-6*H*-purine-6-thione; 3,9-Di-Me, *in* D-60270
6-Mercaptopurine; *S*,3*N*-Di-Me, *in* D-60270
6-Mercaptopurine; *S*,7*N*-Di-Me, *in* D-60270
6-Mercaptopurine; *S*,9*N*-Di-Me, *in* D-60270
1-Methyl-2-methylthio-1*H*-imidazo[4,5-*b*]pyrazine, *in* D-60247
4-Methyl-2-methylthio-4*H*-imidazo[4,5-*b*]pyrazine, *in* D-60247

C_7H_8O
Bicyclo[2.2.1]hept-5-en-2-one, B-80080
Tricyclo[2.2.1.$0^{2,6}$]heptan-3-one, T-70228
3-Vinyl-2-cyclopenten-1-one, V-70011

C_7H_8OS
2,5-Dimethyl-3-thiophenecarboxaldehyde, D-70438
3,5-Dimethyl-2-thiophenecarboxaldehyde, D-70439
2-Mercaptobenzenemethanol, M-80021
3-Mercaptobenzenemethanol, M-80022
4-Mercaptobenzenemethanol, M-80023
2-Thiabicyclo[2.2.2]oct-5-en-3-one, T-60188

$C_7H_8O_2$
2,2-Dimethyl-4-cyclopentene-1,3-dione, D-70395
2,5-Dimethyl-3-furancarboxaldehyde, D-70412
▷ 4,6-Dimethyl-2*H*-pyran-2-one, D-70435
2-Furanpropanal, F-80089
3-Furanpropanal, F-80090
4-Hydroxybenzyl alcohol, H-80114
4-Hydroxy-4-methyl-2,5-cyclohexadien-1-one, H-70169
8-Oxabicyclo[3.2.1]oct-6-en-3-one, O-80051
3-Oxo-1-cyclohexene-1-carboxaldehyde, O-60060
α-Oxo-3-cyclopentene-1-acetaldehyde, O-60061

$C_7H_8O_2S$
2-(Methoxyacetyl)thiophene, *in* H-70103

$C_7H_8O_3$
2,3-Dihydroxybenzyl alcohol, D-80283
2,5-Dihydroxybenzyl alcohol, D-70287
3,4-Dihydroxybenzyl alcohol, D-80284
4,5-Dimethyl-2-furancarboxylic acid, D-70413
4-Hydroxy-2-cyclopentenone; Ac, *in* H-60116
Methyl 3-formylcrotonate, *in* M-70103
2-Methylene-3-oxocyclobutanecarboxylic acid; Me ester, *in* M-80088
5-Oxo-1-cyclohexene-1-carboxylic acid, O-80077
5-Oxo-2-cyclohexene-1-carboxylic acid, O-80078
6-Oxo-1-cyclohexene-1-carboxylic acid, O-80079
3,6,10-Trioxatetracyclo[7.1.0.$0^{2,4}$.$0^{5,7}$]decane, T-80356

$C_7H_8O_4$
Bicyclo[1.1.1]pentane-1,3-dicarboxylic acid, B-80090
3,4-Epoxy-5-hydroxy-1-cyclohexenecarboxylic acid, E-80030
5-Hydroxy-3-methoxy-7-oxabicyclo[4.1.0]hept-3-en-2-one, H-70155
5-(Hydroxymethyl)-1,2,3-benzenetriol, H-80196
5-Hydroxymethyl-2(5*H*)-furanone; Ac, *in* H-60182
3-Methyl-1,2,4,5-benzenetetrol, M-80048
4-Methyl-1,2,3,5-benzenetetrol, M-80049
5-Methyl-1,2,3,4-benzenetetrol, M-80050
Oxysporone, O-70107
Terremutin, T-70009
2-Vinyl-1,1-cyclopropanedicarboxylic acid, V-60011

$C_7H_8O_5$
3,6-Dihydro-2*H*-pyran-2,2-dicarboxylic acid, D-80243
4,5-Dihydroxy-3-oxo-1-cyclohexenecarboxylic acid, D-70328
4-Oxo-2-heptenedioic acid, O-60072
1,4,8-Trioxaspiro[4.5]decane-7,9-dione, *in* O-60084

$C_7H_8O_6$
Aconitic acid; α-Mono-Me ester, *in* A-70055
Aconitic acid; β-Mono-Me ester, *in* A-70055
Aconitic acid; γ-Mono-Me ester, *in* A-70055

C_7H_8S
5,6-Dihydro-4*H*-cyclopenta[*b*]thiophene, D-70180
5,6-Dihydro-4*H*-cyclopenta[*c*]thiophene, D-70181

$C_7H_8S_2$
6,7-Dihydro-5*H*-thieno[3,2-*b*]thiopyran, D-80257
6,7-Dihydro-4*H*-thieno[3,2-*c*]thiopyran, D-80258

C_7H_9Br
2-Bromobicyclo[2.2.1]hept-2-ene, B-80179

$C_7H_9BrO_2$
7-Bromo-5-heptynoic acid, B-60261
2-Bromo-3-methoxy-2-cyclohexen-1-one, *in* B-70201

C_7H_9Cl
5-Chloro-1,3-cycloheptadiene, C-70062

C_7H_9ClO
2-Chloro-2-cyclohepten-1-one, C-60049

$C_7H_9ClO_2$
2-Chloro-3-methoxy-2-cyclohexen-1-one, *in* C-80046

C_7H_9N
4-Heptynenitrile, *in* H-80032
6-Heptynenitrile, *in* H-80033
2-Vinyl-1*H*-pyrrole; *N*-Me, *in* V-60013

C_7H_9NO
7-Azabicyclo[4.2.0]oct-3-en-8-one, A-60331
Bicyclo[2.2.1]hept-5-en-2-one; Oxime, *in* B-80080
Bicyclo[2.2.1]hept-5-en-2-one; Oxime, *in* B-80080
1,2-Dihydro-3*H*-azepin-3-one; 1-Me, *in* D-70171
2,3-Dihydro-1*H*-pyrrolizin-1-ol, D-70261
2,3-Dihydro-1*H*-pyrrolizin-6(5*H*)-one, D-80250
1,5-Dimethyl-1*H*-pyrrole-2-carboxaldehyde, *in* M-70129
3,3*a*,4,6*a*-Tetrahydrocyclopenta[*b*]pyrrol-2(1*H*)-one, T-70048
Tricyclo[2.2.1.$0^{2,6}$]heptan-3-one; Oxime, *in* T-70228

C_7H_9NOS
2-Pyrrolethiolcarboxylic acid; 1-Me, Me ester, *in* P-80226

$C_7H_9NO_2$
3-Amino-5-hydroxybenzyl alcohol, A-60182
2-Amino-6-methoxyphenol, *in* A-70089
5-Amino-2-methoxyphenol, *in* A-70090
Dihydro-1*H*-pyrrolizine-3,5(2*H*,6*H*)-dione, D-70260
2,3-Dimethoxypyridine, *in* H-60223
2,4-Dimethoxypyridine, *in* H-60224
2,6-Dimethoxypyridine, *in* H-60226
3,4-Dimethoxypyridine, *in* H-60227
3-Ethoxy-4(1*H*)-pyridinone, *in* H-60227
Ethyl 1-cyanocyclopropanecarboxylate, *in* C-80196
6-Hydroxy-2(1*H*)-pyridinone; Me ether, *N*-Me, *in* H-60226
2-Methoxy-1-methyl-4(1*H*)-pyridinone, *in* H-60224
3-Methoxy-1-methyl-4(1*H*)-pyridinone, *in* H-60227
3-Methoxy-2-methyl-4(1*H*)-pyridinone, *in* H-80214
4-Methoxy-1-methyl-2(1*H*)-pyridinone, *in* H-60224
5-Methyl-1*H*-pyrrole-2-carboxylic acid; Me ester, *in* M-60124
5-Methyl-1*H*-pyrrole-3-carboxylic acid; Me ester, *in* M-60125
4,5,6,7-Tetrahydro-1,2-benzisoxazol-3(2*H*)-one, T-70037
4,5,6,7-Tetrahydro-2,1-benzisoxazol-3(1*H*)-one, T-70038

$C_7H_9NO_3$
4-Aminodihydro-3-methylene-2-(3*H*)furanone; *N*-Ac, *in* A-70131
3,4-Dihydroxypyridine; Di-Me ether, 1-oxide, *in* H-60227
4,6-Dimethoxy-2(1*H*)-pyridinone, *in* D-70341
3-Hydroxy-1*H*-pyrrole-2-carboxylic acid; Me ether, Me ester, *in* H-80248
4-Hydroxy-1*H*-pyrrole-2-carboxylic acid; Me ether, Me ester, *in* H-80249
4-Hydroxy-1*H*-pyrrole-3-carboxylic acid; Me ether, Me ester, *in* H-80250
5-Methyl-4-isoxazolecarboxylic acid; Et ester, *in* M-80117
7-Oxo-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, O-70079
3-Oxo-2-azabicyclo[2.1.1]hexane-1-carboxylic acid; Me ester, *in* O-80057
2,4-Pyridinediol; Di-Me ether, 1-oxide, *in* H-60224

$C_7H_9NO_4$
5-Oxo-2-pyrrolidinecarboxylic acid; Me ester, *N*-formyl, *in* O-70102

$C_7H_9NO_4S_2$
2,3-Bis(methylsulfonyl)pyridine, *in* P-60218
2,4-Bis(methylsulfonyl)pyridine, *in* M-80029
2,5-Bis(methylsulfonyl)pyridine, *in* P-60220
3,5-Bis(methylsulfonyl)pyridine, *in* P-60222

C_7H_9NS
4-Amino-5,6-dihydro-4*H*-cyclopenta[*b*]thiophene, A-60137
2-(2-Pyridyl)ethanethiol, P-60239
2-(4-Pyridyl)ethanethiol, P-60240

$C_7H_9NS_2$
2,3-Bis(methylthio)pyridine, *in* P-60218
2,4-Bis(methylthio)pyridine, *in* M-80029
2,4-Bis(methylthio)pyridine, *in* P-60219
2,5-Bis(methylthio)pyridine, *in* P-60220
3,5-Bis(methylthio)pyridine, *in* P-60222
1-Methyl-4-(methylthio)-2(1*H*)-pyridinethione, *in* M-80029
1-Methyl-4-(methylthio)-2(1*H*)-pyridinethione, *in* P-60219

$C_7H_9N_2S$
3,5-Dimethyl-2-thiophenecarboxaldehyde; Hydrazone, *in* D-70439

$C_7H_9N_3O$
2-(Hydroxyacetyl)pyridine; Hydrazone, *in* H-70101

$C_7H_9N_3O_3$
5-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Me, *N*(5)-Ac, *in* A-70192

$C_7H_9N_5$
3,7-Dimethyladenine, D-60400
3,9-Dimethyladenine, D-80417
2-(Dimethylamino)purine, *in* A-60243
8-(Dimethylamino)purine, *in* A-60244

C_7H_{10}
Bicyclo[3.1.1]hept-2-ene, B-60087
Bicyclo[4.1.0]hept-3-ene, B-80079
1,2-Bis(methylene)cyclopentane, B-60169
1,3-Bis(methylene)cyclopentane, B-60170
Tricyclo[3.2.0.0^{2,7}]heptane, T-80240
Tricyclo[4.1.0.0^{1,3}]heptane, T-60262

$C_7H_{10}Cl_2O_2$
2,2-Dichloro-6-heptenoic acid, D-80119

$C_7H_{10}INO_2$
5-(Iodomethyl)-2-pyrrolidinone; *N*-Ac, *in* I-80037

$C_7H_{10}N_2O$
2-Oxa-3-azabicyclo[2.2.2]octane; *N*-Cyano, *in* O-70051

$C_7H_{10}N_2O_2$
4,5,6,7-Tetrahydro-3-methoxyisoxazolo[4,5-*c*]pyridine, *in* T-60071
Tetrahydro-1*H*-pyrazolo[1,2-*a*]pyridazine-1,3(2*H*)-dione, T-70088

$C_7H_{10}N_2O_2S$
2-Amino-4-thiazoleacetic acid; Et ester, *in* A-80146
2-Amino-5-thiazoleacetic acid; Et ester, *in* A-80147

$C_7H_{10}N_2O_3$
2-Imidazolidinone; 1,3-Di-Ac, *in* I-70005

$C_7H_{10}N_2O_4$
5-Methyl-3,6-dioxo-2-piperazineacetic acid, M-60064

$C_7H_{10}N_2S$
4,6-Dimethyl-2(1*H*)-pyrimidinethione; 1-Me, *in* D-60450
4-Ethylthio-3-pyridinamine, *in* A-80140
5-Ethylthio-2-pyridinamine, *in* A-80138
6-Ethylthio-3-pyridinamine, *in* A-80141

$C_7H_{10}O$
1-Acetylcyclopentene, A-60028
1-Acetyl-2-methylcyclobutene, A-80028
▷ Bicyclo[2.2.1]heptan-2-one, B-70098
3-Cyclohexene-1-carboxaldehyde, C-70227
3,3-Dimethyl-4-pentynal, D-80467
2,4-Heptadienal, H-60020
1,5-Heptadien-3-one, H-70015
1,5-Heptadien-4-one, H-70016
1,6-Heptadien-3-one, H-70017
4,5-Heptadien-3-one, H-70018
6-Heptyn-2-one, H-70025
4-Methyl-2-cyclohexen-1-one, M-80066
6-Methyl-2-cyclohexen-1-one, M-70059
3-Methyl-1-cyclopentenecarboxaldehyde, M-80067
2-Methylenecyclohexanone, M-80080
3-Methylenecyclohexanone, M-80081
4-Methylenecyclohexanone, M-80082
2-Methylene-7-oxabicyclo[2.2.1]heptane, M-70073
7-Oxatricyclo[4.1.1.0^{2,5}]octane, O-60053
8-Oxatricyclo[3.3.0.0^{2,7}]octane, O-60054
3-Vinyl-2-cyclopenten-1-ol, V-80008

$C_7H_{10}OS$
2-Thiabicyclo[2.2.2]octan-3-one, T-60187

$C_7H_{10}O_2$
1-Carbethoxybicyclo[1.1.0]butane, *in* B-70094
1,1-Diacetylcyclopropane, D-70032
Dihydro-4,4-dimethyl-5-methylene-2(3*H*)-furanone, D-70197
Dihydro-4,5-dimethyl-3-methylene-2(3*H*)-furanone, D-80192
2,2-Dimethyl-1,3-cyclopentanedione, D-70393
4,4-Dimethyl-1,3-cyclopentanedione, D-70394
3,3-Dimethyl-1-cyclopropene-1-carboxylic acid; Me ester, *in* D-60417
6,6-Dimethyl-3-oxabicyclo[3.1.0]hexan-2-one, D-70425
2-Furanpropanol, F-80091
3-Furanpropanol, F-80092
2,4-Heptadienoic acid, H-60021
3-Heptynoic acid, H-80031
4-Heptynoic acid, H-80032
6-Heptynoic acid, H-80033
3,4-Hexadienoic acid; Me ester, *in* H-70037
3,5-Hexadienoic acid; Me ester, *in* H-70038
Hexahydro-1*H*-cyclopenta[*c*]furan-1-one, H-70054
5-Hexynoic acid; Me ester, *in* H-80086
1-Hydroxy-3-cyclohexene-1-carboxaldehyde, H-80146
3-Methoxy-2-cyclohexen-1-one, M-80041
2-Methoxy-3-methyl-2-cyclopenten-1-one, *in* H-60174
3-Methyl-3,5-cyclohexadiene-1,2-diol, M-80063
5-Methyl-2,4-hexadienoic acid, M-70086
5-Methyl-3,4-hexadienoic acid, M-70087
2-Oxocyclohexanecarboxaldehyde, O-80074
3-Oxocyclohexanecarboxaldehyde, O-80075
4-Oxocyclohexanecarboxaldehyde, O-80076
3-Pentyn-2-ol; Ac, *in* P-70041

$C_7H_{10}O_3$
5-Ethyl-3-hydroxy-4-methyl-2(5*H*)-furanone, E-60051
3-Formyl-2,2-dimethyl-1-cyclopropanecarboxylic acid, F-80074
2-Hydroxycyclopentanone; Ac, *in* H-60114
7-Hydroxy-5-heptynoic acid, H-60150
3-Hydroxymethyl-2-methylfuran; Ac, *in* H-80207
4-Hydroxy-3-penten-2-one; Ac, *in* P-60059
4-Methoxy-2,5-dimethyl-3(2*H*)-furanone, *in* H-60120
3-Methyl-4-oxo-2-butenoic acid; Et ester, *in* M-70103
3-Oxocyclopentaneacetic acid, O-70083
2-Oxocyclopentanecarboxylic acid; Me ester, *in* O-70084
4-Oxo-2-hexenoic acid; Me ester, *in* O-80082
4-Oxo-2-pentenoic acid; Et ester, *in* O-70098
2,4,10-Trioxatricyclo[3.3.1.1^{3,7}]decane, T-60377

$C_7H_{10}O_4$
1,1-Cyclopropanedicarboxylic acid; Di-Me ester, *in* C-80196
1,2-Cyclopropanedicarboxylic acid; Di-Me ester, *in* C-70248
Ethyl 3-acetoxyacrylate, *in* O-60090

$C_7H_{10}O_5$
4-Oxoheptanedioic acid, O-60071
3-Oxopentanedioic acid; Di-Me ester, *in* O-60084
1,3,4-Trihydroxy-6-oxabicyclo[3.2.1]octan-7-one, *in* Q-70005

$C_7H_{10}O_6$
1,3-Dioxolane-2,2-diacetic acid, *in* O-60084

$C_7H_{10}S$
Dicyclopropylmethanethione, D-80150
1-Thia-2-cyclooctyne, T-60189
1-Thia-3-cyclooctyne, T-60190

$C_7H_{10}S_5$
4,5-Dimercapto-1,3-dithiole-2-thione; Di-Et thioether, *in* D-80409

$C_7H_{11}ClO$
3,3-Dimethyl-4-pentenoic acid; Chloride, *in* D-60437
4-Methyl-2-hexenoic acid; Chloride, *in* M-80101

$C_7H_{11}ClO_2$
7-Chloro-2-heptenoic acid, C-70069

$C_7H_{11}FO_2$
1-Fluorocyclohexanecarboxylic acid, F-80031

$C_7H_{11}I$
7-Iodo-1,3-heptadiene, I-80032

$C_7H_{11}IO$
2-Iodocycloheptanone, I-70025

$C_7H_{11}N$
2-Azabicyclo[2.2.2]oct-5-ene, A-70279
5-Heptenenitrile, *in* H-70024

$C_7H_{11}NO$
Bicyclo[2.2.1]heptan-2-one; Oxime, *in* B-70098
3-Cyclohexene-1-carboxaldehyde; Oxime, *in* C-70227
4,4-Dimethylglutaraldehydonitrile, *in* D-60434
3,3-Dimethyl-4-pentynal; Oxime, *in* D-80467
Hexahydro-1*H*-pyrrolizin-1-one, H-60057
Hexahydro-3*H*-pyrrolizin-3-one, H-60058
Tetrahydro-1*H*-pyrrolizin-2(3*H*)-one, T-60091

$C_7H_{11}NOS$
4-*tert*-Butyl-2(3*H*)-oxazolethione, B-80288

$C_7H_{11}NO_2$
3,4-Dihydro-2*H*-pyrrole-2-carboxylic acid; Et ester, *in* D-80248
Hexahydro-2(3*H*)-benzoxazolone, H-70052
7-Nitrobicyclo[2.2.1]heptane, N-80037
2-Oxa-3-azabicyclo[2.2.2]octane; *N*-Formyl, *in* O-70051
3-Oxocyclobutanecarboxylic acid; *N*,*N*-Dimethylamide, *in* O-80073
1,2,3,6-Tetrahydro-3-pyridinecarboxylic acid; *N*-Me, *in* T-60084

$C_7H_{11}NO_3$
2-Nitrocycloheptanone, N-80042
5-Oxo-2-pyrrolidinecarboxylic acid; Et ester, *in* O-70102

$C_7H_{11}NO_4$
2-Amino-3-heptenedioic acid, A-60164
2-Amino-5-heptenedioic acid, A-60165

$C_7H_{11}NO_5$
4-Oxoheptanedioic acid; Oxime, *in* O-60071

$C_7H_{11}NS$
4-Mercaptocyclohexanecarbonitrile, *in* M-60020

$C_7H_{11}N_3O_2$
3-Amino-5-methyl-1*H*-pyrazole-4-carboxylic acid; Et ester, *in* A-80110
4-Amino-5-methyl-1*H*-pyrazole-3-carboxylic acid; Et ester, *in* A-80111
3-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Me, Et ester, *in* A-70187
3-Amino-1*H*-pyrazole-5-carboxylic acid; *N*(1)-Me, Et ester, *in* A-70188
5-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Me, Et ester, *in* A-70192

$C_7H_{11}N_3O_2S$
5-Mercapto-1-methylhistidine, *in* M-80025
Ovothiol *A*, O-70050

C_7H_{12}
4,4-Dimethyl-2-pentyne, D-60438

$C_7H_{12}BrO_2$
2-(4-Bromobutyl)-1,3-dioxole, *in* B-70263

$C_7H_{12}Br_2$
1,1-Dibromocycloheptane, D-60091
1,1-Dibromo-2,2,3,3-tetramethylcyclopropane, D-80103

$C_7H_{12}Br_2O$
2,4-Dibromo-2,4-dimethyl-3-pentanone, D-60099

$C_7H_{12}Br_2O_2$
1,1-Dibromo-3,3-dimethoxy-2-methyl-1-butene, *in* D-70094

$C_7H_{12}ClN$
8-Azabicyclo[3.2.1]octane; *N*-Chloro, *in* A-70278

$C_7H_{12}ClNO_4$
1,2,3,5,6,7-Hexahydropyrrolizinium(1+); Perchlorate, *in* H-70071

$C_7H_{12}N^{\oplus}$
1,2,3,5,6,7-Hexahydropyrrolizinium(1+), H-70071

$C_7H_{12}N_2$
3(5)-*tert*-Butylpyrazole, B-80291
4-*tert*-Butylpyrazole, B-80292

$C_7H_{12}N_2O$
3,5-Dihydro-3,3,5,5-tetramethyl-4*H*-pyrazol-4-one, D-60286
Hexahydro-1*H*-pyrrolizin-1-one; Oxime, *in* H-60057

$C_7H_{12}N_2OS$
3,5-Dihydro-3,3,5,5-tetramethyl-4*H*-pyrazole-4-thione; *S*-Oxide, *in* D-60285

$C_7H_{12}N_2O_2$
5-Amino-3,4-dihydro-2*H*-pyrrole-2-carboxylic acid; Et ester, *in* A-70135
1-Oxa-2-azaspiro[2,5]octane; *N*-Carbamoyl, *in* O-70052

$C_7H_{12}N_2O_4$
2,6-Diamino-3-heptenedioic acid, D-60036

$C_7H_{12}N_2O_5$
N,N'-Carbonylbisglycine; Di-Me ester, *in* C-80020

$C_7H_{12}N_2S$
3,5-Dihydro-3,3,5,5-tetramethyl-4*H*-pyrazole-4-thione, D-60285

$C_7H_{12}N_4O$
Caffeidine, C-60003

$C_7H_{12}O$
2,3-Dimethyl-3,4-dihydro-2*H*-pyran, D-70398
3,3-Dimethyl-4-penten-2-one, D-70429
4,4-Dimethyl-1-pentyn-3-ol, D-80468
2,4-Heptadien-1-ol, H-70014
1-Methoxycyclohexene, M-60037
1-Methyl-2-cyclohexen-1-ol, M-80065
6-Methyl-2-cyclohexen-1-ol, M-70058
2-Methyl-4-hexenal, M-80098
3-Methyl-4-hexen-2-one, M-80115
1-Methyl-7-oxabicyclo[4.1.0]heptane, M-80125
3,6,7,8-Tetrahydro-2*H*-oxocin, T-60076

$C_7H_{12}OS$
2-Hexyl-5-methyl-3(2*H*)furanone; *S*-Oxide (*exo*-), *in* H-60079
2-(Methylthio)cyclohexanone, *in* M-70025
3-(Methylthio)cyclohexanone, *in* M-70026
4-Methylthiocyclohexanone, *in* M-70027
2,2,4,4-Tetramethyl-3-thietanone, T-60154
3,3,4,4-Tetramethyl-2-thietanone, T-60155

$C_7H_{12}O_2$
2-Cycloheptene-1,4-diol, C-80179
2,3-Dimethylcyclopropanol; Ac, *in* D-70397
2,2-Dimethyl-4-oxo-1-pentanal, D-80464
3,3-Dimethyl-4-pentenoic acid, D-60437
5-Heptenoic acid, H-70024
5-Hydroxy-2-methylcyclohexanone, H-70171
2-Methylhexanedial, M-80096
2-Methyl-4-hexenoic acid, M-80100
4-Methyl-2-hexenoic acid, M-80101
4-Oxoheptanal, O-60070
Tetrahydro-5,6-dimethyl-2*H*-pyran-2-one, T-70059

$C_7H_{12}O_2S$
3-(Ethylthio)-2-propenoic acid; Et ester, *in* E-60055
4-Mercaptocyclohexanecarboxylic acid, M-60020
3-Oxobutanethioic acid; Isopropyl ester, *in* O-70080

$C_7H_{12}O_3$
4-Acetyl-2,2-dimethyl-1,3-dioxolane, A-70042
▷ Botryodiplodin, B-60194
3,3-Dimethyl-4-oxopentanoic acid, D-60433
4,4-Dimethyl-5-oxopentanoic acid, D-60434
2-Hydroxycyclohexanecarboxylic acid, H-70119
5-Hydroxy-3-methyl-2-pentenoic acid; Me ester, *in* H-80211
3-Methyl-2-oxobutanoic acid; Et ester, *in* M-80129
3-Oxopropanoic acid; *tert*-Butyl ester, *in* O-60090

$C_7H_{12}O_3S$
2-(Methylsulfonyl)cyclohexanone, *in* M-70025
2,2,4,4-Tetramethyl-3-thietanone; 1,1-Dioxide, *in* T-60154

$C_7H_{12}O_4$
(1-Methylpropyl)propanedioic acid, M-70119
▷ 1,2-Propanediol; Di-Ac, *in* P-70118

$C_7H_{12}O_5$
▷ 1,3-Diacetylglycerol, D-60023
2-Hydroxy-2-isopropylbutanedioic acid, H-60165
2-Hydroxy-3-isopropylbutanedioic acid, H-60166
5-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol, H-70172

$C_7H_{12}O_6$
Quinic acid, Q-70005

$C_7H_{12}S$
Hexahydro-2*H*-cyclopenta[*b*]thiophene, H-60049

$C_7H_{13}Br$
6-Bromo-1-heptene, B-80208
7-Bromo-1-heptene, B-60260
3-Bromo-1,1,2,2-tetramethylcyclopropane, B-80261

$C_7H_{13}ClO$
4,4-Dimethylpentanoic acid; Chloride, *in* D-70428

$C_7H_{13}ClO_2$
1-Chloro-3-pentanol; Ac, *in* C-70138

$C_7H_{13}FO$
2-Fluoroheptanal, F-60034

$C_7H_{13}I$
5-Iodo-4,4-dimethyl-1-pentene, I-80023
6-Iodo-1-heptene, I-70035
7-Iodo-1-heptene, I-70036

$C_7H_{13}IO_2$
1-Iodo-5,5-dimethoxypentene, *in* I-70052
5-Iodo-2-pentanol; Ac, *in* I-60056
2-(3-Iodopropyl)-2-methyl-1,3-dioxolane, *in* I-60057

$C_7H_{13}N$
1-Aminobicyclo[2.2.1]heptane, A-80060
7-Aminobicyclo[2.2.1]heptane, A-80061
7-Azabicyclo[4.2.0]octane, A-70277
8-Azabicyclo[3.2.1]octane, A-70278
4,4-Dimethylpentanoic acid; Nitrile, *in* D-70428
▷ 2-Propyn-1-amine; *N*-Di-Et, *in* P-60184

$C_7H_{13}NO$
2-Acetylpiperidine, A-70051
3,3-Dimethyl-4-penten-2-one; Oxime, *in* D-70429
Hexahydro-4(1*H*)-azocinone, H-70047
Hexahydro-5(2*H*)-azocinone, H-70048

$C_7H_{13}NOS$
Hexahydro-1,5-thiazonin-6(7*H*)-one, H-70075
4-Mercaptocyclohexanecarboxylic acid; Amide, *in* M-60020

$C_7H_{13}NOS_2$
1-Isothiocyanato-5-(methylsulfinyl)pentene, *in* I-60140

$C_7H_{13}NO_2$
2-Amino-2-hexenoic acid; Me ester, *in* A-60167
3-Amino-4-hexenoic acid; Me ester, *in* A-60171
2-Hydroxycyclohexanecarboxylic acid; Amide, *in* H-70119
2-Methyl-2-piperidinecarboxylic acid, M-60119
Nitrocycloheptane, N-60025
3-Piperidinecarboxylic acid; Me ester, *in* P-70102
Stachydrine, S-60050

$C_7H_{13}NO_3$
4,4-Dimethyl-5-oxopentanoic acid; Oxime, *in* D-60434
3-Methyl-2-oxobutanoic acid; Et ester, oxime, *in* M-80129

$C_7H_{13}NO_4$
L-Allothreonine; Ac, Me ether, *in* T-60217
2-Amino-2-isopropylbutanedioic acid, A-60212
2-Amino-3-isopropylbutanedioic acid, A-70162
2-Amino-3-propylbutanedioic acid, A-70186
Detoxinine, D-80040
2-Hydroxy-2-isopropylsuccinamic acid, *in* H-60165

$C_7H_{13}NO_4S$
Isobuteine, I-80049

$C_7H_{13}NO_6S$
3-[(2-Carboxypropyl)sulfonyl]alanine, *in* I-80049

$C_7H_{13}NS$
4,5-Dihydro-2-(1-methylpropyl)thiazole, D-70224

$C_7H_{13}NS_2$
1-Isothiocyanato-5-(methylthio)pentane, I-60140

$C_7H_{13}N_3$
6*bH*-2*a*,4*a*,6*a*-Hexahydrotriazacyclopenta[*cd*]pentalene, H-70077

$C_7H_{13}N_3O_4$
N-Asparaginylalanine, A-60310

C_7H_{14}
tert-Butylcyclopropane, B-80285

$C_7H_{14}BrN$
2-(Bromomethyl)cyclohexanamine, B-70239

$C_7H_{14}Br_2$
1,5-Dibromo-3,3-dimethylpentane, D-70090

$C_7H_{14}N_2$
1,4-Diazabicyclo[4.3.0]nonane, D-60054
Diisopropylcyanamide, D-60392
6-Heptyne-2,5-diamine, H-60026
Hexahydro-1*H*-pyrazolo[1,2-*a*]pyridazine, H-70067
Octahydropyrrolo[3,4-*c*]pyrrole; *N*-Me, *in* O-70017

$C_7H_{14}N_2O$
2-Acetylpiperidine; Oxime (*E*-), *in* A-70051
2-Imidazolidinone; 1-*tert*-Butyl, *in* I-70005
3,3,5,5-Tetramethyl-4-pyrazolidinone, T-60153

$C_7H_{14}N_2O_2$
2-Hydroxycyclohexanecarboxylic acid; Hydrazide, *in* H-70119

$C_7H_{14}N_2O_3$
2-Hydroxy-2-isopropylsuccinamide, *in* H-60165

$C_7H_{14}N_2O_3S$
S-(2-Aminoethyl)cysteine; N^{α}-Ac, *in* A-60152
S-(2-Aminoethyl)cysteine; N^{ϵ}-Ac, *in* A-60152

$C_7H_{14}N_2O_6$
N-Carbamoylglucosamine, C-70015

$C_7H_{14}N_2O_6S$
γ-Glutamyltaurine, G-60027

$C_7H_{14}N_4O_5$
3,3-Bis(methylnitraminomethyl)oxetane, *in* B-60140

$C_7H_{14}O$
1-Methoxy-1-hexene, M-70046
4-Methoxy-2-hexene, *in* H-60077
4-Methyl-3-hexanone, M-80097
2-Methyl-4-hexen-1-ol, M-80102
2-Methyl-4-hexen-2-ol, M-80103
2-Methyl-5-hexen-1-ol, M-80104
3-Methyl-5-hexen-1-ol, M-80105
4-Methyl-2-hexen-1-ol, M-80106
4-Methyl-3-hexen-2-ol, M-80107
4-Methyl-4-hexen-1-ol, M-80108
4-Methyl-4-hexen-2-ol, M-80109
4-Methyl-5-hexen-1-ol, M-80110
5-Methyl-4-hexen-2-ol, M-80111
5-Methyl-4-hexen-3-ol, M-80112
5-Methyl-5-hexen-1-ol, M-80113
5-Methyl-5-hexen-3-ol, M-80114

$C_7H_{14}OS_2$
1,5-Dithionane; 1-Oxide, *in* D-70526

$C_7H_{14}O_2$
3,4-Dimethylpentanoic acid, D-60435
4,4-Dimethylpentanoic acid, D-70428
2-Hydroxycyclohexanemethanol, H-70120
3-Hydroxy-4,4-dimethyl-2-pentanone, H-80154
3-Methyl-1,2-cyclohexanediol, M-80064

$C_7H_{14}O_3$
5,5-Dimethoxy-2-pentanone, *in* O-60083
2-Hydroxy-2-methylhexanoic acid, H-60184
2-Hydroxy-3-methylhexanoic acid, H-60185
3-Hydroxy-2-methylpentanoic acid; Me ester, *in* H-80209
2-Hydroxy-2,3,3-trimethylbutanoic acid, H-80262

$C_7H_{14}O_3S$
2-Mercaptopropanoic acid; Et ester, *S*-Ac, *in* M-60027

$C_7H_{14}O_4$
5,6-Dihydroxyhexanoic acid; Me ester, *in* D-60329
Glycerol 1-acetate; Di-Me ether, *in* G-60029

$C_7H_{14}O_5$
5-(Hydroxymethyl)-1,2,3,4-cyclohexanetetrol, H-70170

$C_7H_{14}S_2$
1,1-Cyclopentanedimethanethiol, C-70243
1,5-Dithionane, D-70526

$C_7H_{15}N$
5-Hexen-1-amine; *N*-Me, *in* H-80078
5-Methyl-4-hexen-1-amine, M-80099
▷ Octahydroazocine, O-70010
1,2,2,3,3-Pentamethylaziridine, *in* T-80139
1,2,5-Trimethylpyrrolidine, *in* D-70437

$C_7H_{15}NO$
2-(Aminomethyl)cyclohexanol, A-70169
4,4-Dimethylpentanoic acid; Amide, *in* D-70428
3-Piperidineethanol, P-70103

$C_7H_{15}NO_2$
2-Amino-2,3-dimethylbutanoic acid; Me ester, *in* A-60148
2-Amino-3,3-dimethylbutanoic acid; Me ester, *in* A-70136
2-Amino-4,4-dimethylpentanoic acid, A-70137
2-Amino-2-methylbutanoic acid; Et ester, *in* A-70167
4-Nitroheptane, N-60027

$C_7H_{15}NO_3$
3-Amino-2-hydroxy-5-methylhexanoic acid, A-60188
Carnitine, C-70024
N-(2,3-Dihydroxy-3-methylbutyl)acetamide, *in* A-60216
3-Nitro-1-propanol; *tert*-Butyl ether, *in* N-60039

$C_7H_{15}NO_4$
1,1-Diethoxy-3-nitropropane, *in* N-60037

$C_7H_{15}NS$
3-Aminotetrahydro-2*H*-thiopyran; *N,N*-Di-Me, *in* A-70200
2-Pyrrolidinemethanethiol; 1-Et, *in* P-70185

$C_7H_{15}N_2O^{\oplus}$
3-Cyano-2-hydroxy-*N,N,N*-trimethylpropanaminium, *in* C-70024

$C_7H_{15}N_3O_3$
N-Ornithylglycine, O-70047

$C_7H_{16}N_2O_3S$
Aminoiminomethanesulfonic acid; *N,N*-Diisopropyl, *in* A-60210

$C_7H_{16}N_4O_2$
Blastidic acid, B-80170

$C_7H_{16}O$
3,4-Dimethyl-1-pentanol, D-60436

$C_7H_{16}O_2$
2,4-Dimethyl-1,3-pentanediol, D-80466
1,5-Heptanediol, H-80030

$C_7H_{16}S$
3-Ethyl-3-pentanethiol, E-60053

$C_7H_{16}S_2$
3,3-Dimethyl-1,5-pentanedithiol, D-70427
1,7-Heptanedithiol, H-70023

$C_7H_{17}N_3O_4S$
N-Ornithyltaurine, O-60042

$C_8F_4O_3$
4,5,6,7-Tetrafluoro-1,3-isobenzofurandione, *in* T-70031

C_8F_{12}
Dodecafluorobicyclobutylidene, D-60513

$C_8F_{12}S_2$
2,4-Bis[2,2,2-Trifluoro-1-(trifluoromethyl)ethylidene]-1,3-dithietane, B-60188

$C_8H_2ClF_5O$
Pentafluorophenylacetic acid; Chloride, *in* P-80027

$C_8H_2F_4O_4$
2,3,5,6-Tetrafluoro-1,4-benzenedicarboxylic acid, T-70029
2,4,5,6-Tetrafluoro-1,3-benzenedicarboxylic acid, T-70030
3,4,5,6-Tetrafluoro-1,2-benzenedicarboxylic acid, T-70031

$C_8H_2F_5N$
Pentafluorophenylacetonitrile, *in* P-80027

$C_8H_2O_2S_4$
Benzo[1,2-*d*:4,5-*d'*]bis[1,3]dithiole-2,6-dione, B-70028

$C_8H_3Br_4N$
4,5,6,7-Tetrabromo-2*H*-isoindole, T-80013

$C_8H_3Cl_2F_3N_2$
▷ 4,5-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60157
▷ 4,6-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60158
▷ 4,7-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60159
▷ 5,6-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole, D-60160

$C_8H_3Cl_2NO_4$
2-Nitro-1,3-benzenedicarboxylic acid; Dichloride, *in* N-80035

$C_8H_3Cl_4N$
4,5,6,7-Tetrachloro-2*H*-isoindole, T-80017

$C_8H_3FO_2$
3-Fluorobenzocyclobutene-1,2-dione, F-80021

$C_8H_3F_4N_3O$
4,5,6,7-Tetrafluoro-1*H*-benzotriazole; 1-Ac, *in* T-70035

$C_8H_3F_5O_2$
Pentafluorophenylacetic acid, P-80027

$C_8H_3NO_6$
3-Hydroxy-6-nitro-1,2-benzenedicarboxylic acid; Anhydride, *in* H-70189
4-Hydroxy-5-nitro-1,2-benzenedicarboxylic acid; Anhydride, *in* H-70191

$C_8H_4Br_2O$
2,3-Dibromobenzofuran, D-60086
5,7-Dibromobenzofuran, D-60087

$C_8H_4Br_6$
1,2,3,4-Tetrabromo-5,6-bis(bromomethyl)benzene, T-80012

$C_8H_4ClF_3O$
2-Chloro-3-(trifluoromethyl)benzaldehyde, C-70164
2-Chloro-5-(trifluoromethyl)benzaldehyde, C-70165
2-Chloro-6-(trifluoromethyl)benzaldehyde, C-70166
4-Chloro-3-(trifluoromethyl)benzaldehyde, C-70167
5-Chloro-2-(trifluoromethyl)benzaldehyde, C-70168

$C_8H_4Cl_2N_2$
1,4-Dichlorophthalazine, D-60148
▷ 2,3-Dichloroquinoxaline, D-60150

$C_8H_4Cl_2N_2O$
2,3-Dichloroquinoxaline; 1-Oxide, *in* D-60150

$C_8H_4Cl_2O$
2,3-Dichlorobenzofuran, D-60125
5,7-Dichlorobenzofuran, D-60126

$C_8H_4Cl_2O_2$
4,6-Dichloro-1,3-benzenedicarboxaldehyde, D-60118

$C_8H_4FN_3O_5$
5-Fluoro-2,4-dinitroaniline; *N*-Ac, *in* F-60031

$C_8H_4F_4O_2$
2,3,4,5-Tetrafluorobenzoic acid; Me ester, *in* T-70032

$C_8H_4F_5NO$
Pentafluorophenylacetic acid; Amide, *in* P-80027

$C_8H_4F_6$
1,2-Bis(trifluoromethyl)benzene, B-60175
1,3-Bis(trifluoromethyl)benzene, B-60176
1,4-Bis(trifluoromethyl)benzene, B-60177

$C_8H_4N_2O$
2-Cyanofuro[2,3-*b*]pyridine, *in* F-60098
2-Cyanofuro[3,2-*b*]pyridine, *in* F-60100
3-Cyanofuro[2,3-*b*]pyridine, *in* F-60099
3-Cyanofuro[3,2-*b*]pyridine, *in* F-60101
2-Cyanofuro[2,3-*c*]pyridine, *in* F-60102
2-Cyanofuro[3,2-*c*]pyridine, *in* F-60104
3-Cyanofuro[2,3-*c*]pyridine, *in* F-60103
3-Cyanofuro[3,2-*c*]pyridine, *in* F-60105

$C_8H_4N_2O_2$
5,8-Quinoxalinedione, Q-60010

$C_8H_4N_2O_5$
4-Amino-5-nitro-1,2-benzenedicarboxylic acid; Anhydride, *in* A-70177
3-Cyano-2-hydroxy-5-nitrobenzoic acid, *in* H-70188

$C_8H_4N_4O$
Furazano[3,4-*b*]quinoxaline, F-70051

$C_8H_4N_4O_2$
Furoxano[3,4-*b*]quinoxaline, *in* F-70051

$C_8H_4OS_2$
3-Thioxo-1(3*H*)-benzo[*c*]thiophenone, T-80192

$C_8H_4O_2S$
3-Thioxo-1(3*H*)-isobenzofuranone, T-80193

$C_8H_4O_4$
2,2′-Bifurylidene-5,5′-dione, B-80094
3,4-Dihydroxybenzocyclobutene-1,2-dione, D-80274
3,5-Dihydroxybenzocyclobutene-1,2-dione, D-80275
3,6-Dihydroxybenzocyclobutene-1,2-dione, D-80276
4,5-Dihydroxybenzocyclobutene-1,2-dione, D-80277

$C_8H_4O_6$
1,4-Benzoquinone-2,3-dicarboxylic acid, B-70047
1,4-Benzoquinone-2,5-dicarboxylic acid, B-70048
1,4-Benzoquinone-2,6-dicarboxylic acid, B-70049

C_8H_4S
▷ 2,5-Diethynylthiophene, D-80157

$C_8H_5BrN_2$
1-Bromophthalazine, B-70266
5-Bromophthalazine, B-70267
6-Bromophthalazine, B-70268

C_8H_5BrOS
2-Bromobenzo[*b*]thiophene; 1-Oxide, *in* B-60204
3-Bromobenzo[*b*]thiophene; 1-Oxide, *in* B-60205

$C_8H_5BrO_2$
4-Bromo-1(3*H*)-isobenzofuranone, B-70224
7-Bromo-1(3*H*)-isobenzofuranone, B-70225

$C_8H_5BrO_2S$
2-Bromobenzo[*b*]thiophene; 1,1-Dioxide, *in* B-60204
3-Bromobenzo[*b*]thiophene; 1,1-Dioxide, *in* B-60205
4-Bromobenzo[*b*]thiophene; 1,1-Dioxide, *in* B-60206
5-Bromobenzo[*b*]thiophene; 1,1-Dioxide, *in* B-60207
6-Bromobenzo[*b*]thiophene; 1,1-Dioxide, *in* B-60208

C_8H_5BrS
2-Bromobenzo[*b*]thiophene, B-60204
3-Bromobenzo[*b*]thiophene, B-60205
4-Bromobenzo[*b*]thiophene, B-60206
5-Bromobenzo[*b*]thiophene, B-60207
6-Bromobenzo[*b*]thiophene, B-60208
7-Bromobenzo[*b*]thiophene, B-60209

$C_8H_5Br_3O$
2′,3′,5′-Tribromoacetophenone, T-80216

$C_8H_5ClN_2$
1-Chlorophthalazine, C-70148
5-Chlorophthalazine, C-70149
6-Chlorophthalazine, C-70150
N-Cyanobenzenecarboximidoyl chloride, C-80168

C_8H_5ClOS
2-Chlorobenzo[*b*]thiophene; 1-Oxide, *in* C-60042
3-Chlorobenzo[*b*]thiophene; 1-Oxide, *in* C-60043

$C_8H_5ClO_2$
4-Chloro-1(3*H*)-isobenzofuranone, C-70079
7-Chloro-1(3*H*)-isobenzofuranone, C-70080

$C_8H_5ClO_2S$
2-Chlorobenzo[*b*]thiophene; 1,1-Dioxide, *in* C-60042
3-Chlorobenzo[*b*]thiophene; 1,1-Dioxide, *in* C-60043
7-Chlorobenzo[*b*]thiophene; 1,1-Dioxide, *in* C-60047

C_8H_5ClS
2-Chlorobenzo[*b*]thiophene, C-60042
3-Chlorobenzo[*b*]thiophene, C-60043
4-Chlorobenzo[*b*]thiophene, C-60044
5-Chlorobenzo[*b*]thiophene, C-60045
6-Chlorobenzo[*b*]thiophene, C-60046
7-Chlorobenzo[*b*]thiophene, C-60047

$C_8H_5Cl_3O$
2,2,2-Trichloroacetophenone, T-70219

C_8H_5FO
6-Fluorobenzocyclobuten-1-one, F-80022

$C_8H_5FO_2$
4-Fluoro-1(3*H*)-isobenzofuranone, F-70027
7-Fluoro-1(3*H*)-isobenzofuranone, F-70028

$C_8H_5F_3$
(Trifluoroethenyl)benzene, T-80275

$C_8H_5F_3N_2$
2-(Trifluoromethyl)-1*H*-benzimidazole, T-60287

$C_8H_5F_3O_2$
4-Hydroxy-2-(trifluoromethyl)benzaldehyde, H-70228
4-Hydroxy-3-(trifluoromethyl)benzaldehyde, H-70229
Phenyl trifluoroacetate, *in* T-80267
2,4,5-Trifluorobenzoic acid; Me ester, *in* T-70240

$C_8H_5F_5O$
1-(Pentafluorophenyl)ethanol, P-60040

C_8H_5I
▷ 1-Iodo-2-phenylacetylene, I-70055

$C_8H_5IO_2$
4-Iodo-1(3*H*)-isobenzofuranone, I-70044
7-Iodo-1(3*H*)-isobenzofuranone, I-70045

C_8H_5NO
3*H*-Indol-3-one, I-60035

$C_8H_5NOS_2$
2-Thiazolyl 2-thienyl ketone, T-80174

$C_8H_5NO_2$
Furo[2,3-*b*]pyridine-2-carboxaldehyde, F-60093
Furo[2,3-*b*]pyridine-3-carboxaldehyde, F-60094
Furo[3,2-*b*]pyridine-2-carboxaldehyde, F-60095
Furo[2,3-*c*]pyridine-2-carboxaldehyde, F-60096
Furo[3,2-*c*]pyridine-2-carboxaldehyde, F-60097
3-Imino-1(3*H*)-isobenzofuranone, I-80009
Isatogen, *in* I-60035

$C_8H_5NO_2S$
2*H*-1,3-Benzothiazine-2,4(3*H*)-dione, B-80041
2*H*-1,4-Benzothiazine-2,3(4*H*)-dione, B-70054
2*H*-3,1-Benzothiazine-2,4(1*H*)-dione, B-80042
1,2-Dihydro-2-thioxo-4*H*-3,1-benzoxazin-4-one, D-80261
2-Furyl 2-thiazolyl ketone, F-80098

$C_8H_5NO_3$
Furo[2,3-*b*]pyridine-2-carboxylic acid, F-60098
Furo[2,3-*b*]pyridine-3-carboxylic acid, F-60099
Furo[3,2-*b*]pyridine-2-carboxylic acid, F-60100
Furo[3,2-*b*]pyridine-3-carboxylic acid, F-60101
Furo[2,3-*c*]pyridine-2-carboxylic acid, F-60102
Furo[2,3-*c*]pyridine-3-carboxylic acid, F-60103
Furo[3,2-*c*]pyridine-2-carboxylic acid, F-60104
Furo[3,2-*c*]pyridine-3-carboxylic acid, F-60105

$C_8H_5NO_6$
2-Nitro-1,3-benzenedicarboxylic acid, N-80035

$C_8H_5NO_7$
2-Hydroxy-5-nitro-1,3-benzenedicarboxylic acid, H-70188
3-Hydroxy-6-nitro-1,2-benzenedicarboxylic acid, H-70189
4-Hydroxy-3-nitro-1,2-benzenedicarboxylic acid, H-70190
4-Hydroxy-5-nitro-1,2-benzenedicarboxylic acid, H-70191
4-Hydroxy-5-nitro-1,3-benzenedicarboxylic acid, H-70192

$C_8H_5NS_3$
3-Phenyl-1,4,2-dithiazole-5-thione, P-60088

$C_8H_5N_2O$
3-Hydroxyiminoindole, *in* I-60035

$C_8H_5N_3O_2$
5-Nitrophthalazine, N-70062

$C_8H_5N_3O_8$
2,4,6-Trinitrobenzoic acid; Me ester, *in* T-70303

$C_8H_5N_3O_9$
3-Hydroxy-5-methyl-2,4,6-trinitrobenzoic acid, H-60193

$C_8H_5N_3S$
1-Thia-5,8,8*b*-triazaacenaphthylene, T-80169

$C_8H_5N_5$
Tetrazolo[5,1-*a*]phthalazine, T-70155

$C_8H_5N_5O_9$
2,3,4,6-Tetranitroacetanilide, *in* T-60159

C_8H_6
Cubene, C-80160
1,3,5-Cyclooctatrien-7-yne, C-70240

$C_8H_6BrFO_2$
2-Bromo-4-fluorobenzoic acid; Me ester, *in* B-60240

$C_8H_6BrNO_4$
4-(Bromomethyl)-2-nitrobenzoic acid, B-60297

$C_8H_6Br_2I_2O_2$
1,2-Dibromo-3,6-diiodo-4,5-dimethoxybenzene, *in* D-80090

C_8H_6ClNS
2-Chloro-6-(methylthio)benzonitrile, *in* C-70082

$C_8H_6Cl_2O_2$
2,6-Dichloro-4-methoxybenzaldehyde, *in* D-70121

$C_8H_6Cl_2O_3$
2,3-Dichloro-4-methoxybenzoic acid, *in* D-60133

$C_8H_6FIO_2$
3-Fluoro-2-iodobenzoic acid; Me ester, *in* F-70021

C_8H_6FN
3-Fluoro-1*H*-indole, F-80043
4-Fluoro-1*H*-indole, F-80044
5-Fluoro-1*H*-indole, F-80045
6-Fluoro-1*H*-indole, F-80046
7-Fluoro-1*H*-indole, F-80047

C_8H_6FNS
2-Fluoro-6-(methylthio)benzonitrile, *in* F-70030

$C_8H_6FN_3O_5$
6-Fluoro-3,4-dinitroaniline; *N*-Ac, *in* F-60032

$C_8H_6F_3NO_3$
1-Methoxy-2-nitro-4-(trifluoromethyl)benzene, *in* N-60048
1-Methoxy-3-nitro-5-(trifluoromethyl)benzene, *in* N-60052
1-Methoxy-4-nitro-2-(trifluoromethyl)benzene, *in* N-60053
4-Methoxy-1-nitro-2-(trifluoromethyl)benzene, *in* N-60054

C_8H_6IN
7-Iodo-1*H*-indole, I-70043

$C_8H_6I_2$
1,4-Diiodopentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane, D-70359

$C_8H_6N_2O$
2-(2-Oxazolyl)pyridine, O-70071
2-(5-Oxazolyl)pyridine, O-70072
3-(2-Oxazolyl)pyridine, O-70073

3-(5-Oxazolyl)pyridine, O-70074
4-(2-Oxazolyl)pyridine, O-70075
4-(5-Oxazolyl)pyridine, O-70076

$C_8H_6N_2OS$
2,3-Dihydro-2-thioxo-4(1*H*)-quinazolinone, D-60296
2,3-Dihydro-4-thioxo-2(1*H*)-quinazolinone, D-60295

$C_8H_6N_2OSe$
2,3-Dihydro-2-selenoxo-4(1*H*)-quinazolinone, D-60281
3,4-Dihydro-4-selenoxo-2(1*H*)-quinazolinone, D-60280

$C_8H_6N_2O_2$
1,4-Dihydro-2,3-quinoxalinedione, D-60279
Furo[2,3-*b*]pyridine-2-carboxaldehyde; Oxime, *in* F-60093
Furo[3,2-*b*]pyridine-2-carboxaldehyde; Oxime, *in* F-60095
Furo[2,3-*c*]pyridine-2-carboxaldehyde; Oxime, *in* F-60096
Furo[3,2-*c*]pyridine-2-carboxaldehyde; Oxime, *in* F-60097
Furo[2,3-*b*]pyridine-3-carboxylic acid; Amide, *in* F-60099
Furo[3,2-*b*]pyridine-3-carboxylic acid; Amide, *in* F-60101
Furo[2,3-*c*]pyridine-3-carboxylic acid; Amide, *in* F-60103
Furo[3,2-*c*]pyridine-3-carboxylic acid; Amide, *in* F-60105
3*H*-Indol-3-one; 1-Oxide, oxime, *in* I-60035
5-Nitro-1*H*-indole, N-70052
5,8-Quinazolinediol, Q-60002
5,8-Quinoxalinediol, Q-60008
6,7-Quinoxalinediol, Q-60009

$C_8H_6N_2O_3$
1,2,4-Oxadiazolidine-3,5-dione; 2-Ph, *in* O-70060
1,2,4-Oxadiazolidine-3,5-dione; 4-Ph, *in* O-70060

$C_8H_6N_2O_4$
DDED, *in* E-60049

$C_8H_6N_2O_5$
2-Nitro-1,3-benzenedicarboxylic acid; Monoamide, *in* N-80035

$C_8H_6N_2O_6$
3-Amino-4-nitro-1,2-benzenedicarboxylic acid, A-70174
3-Amino-6-nitro-1,2-benzenedicarboxylic acid, A-70175
4-Amino-3-nitro-1,2-benzenedicarboxylic acid, A-70176
4-Amino-5-nitro-1,2-benzenedicarboxylic acid, A-70177
5-Amino-3-nitro-1,2-benzenedicarboxylic acid, A-70178
2,6-Dinitrobenzoic acid; Me ester, *in* D-60457
3,5-Dinitrobenzoic acid; Me ester, *in* D-60458

$C_8H_6N_2S$
2-(1*H*)-Quinoxalinethione, Q-80004

$C_8H_6N_4O_7$
2,4,6-Trinitroacetanilide, *in* T-70301

C_8H_6O
Cyclopenta[*c*]pyran, C-80192

C_8H_6OS
Benzo[*b*]thiophen-3(2*H*)-one, B-60048
1(3*H*)-Isobenzofuranthione, I-70063

$C_8H_6O_2$
Bicyclo[2.2.2]octa-5,7-diene-2,3-dione, B-70109
▷ Bicyclo[4.2.0]octa-1,5-diene-3,4-dione, B-70110

$C_8H_6O_3$
4*H*-1,3-Benzodioxin-2-one, B-60028
3,6-Dihydroxybenzocyclobuten-1-one, D-80278
4,5-Dihydroxybenzocyclobuten-1-one, D-80279
4,6-Dihydroxybenzocyclobuten-1-one, D-80280
5,6-Dihydroxybenzocyclobuten-1-one, D-80281
2-Hydroxy-3(2*H*)-benzofuranone, H-80107
4-Hydroxy-3(2*H*)-benzofuranone, H-80108
5-Hydroxy-3(2*H*)-benzofuranone, H-80109
6-Hydroxy-3(2*H*)-benzofuranone, H-80110
7-Hydroxy-3(2*H*)-benzofuranone, H-80111

$C_8H_6O_3S$
Benzo[*b*]thiophen-3(2*H*)-one; 1,1-Dioxide, *in* B-60048

$C_8H_6O_4$
1,2-Benzoquinone-3-carboxylic acid; Me ester, *in* B-70045
1,2-Benzoquinone-4-carboxylic acid; Me ester, *in* B-70046
2,3-Dihydro-1,4-benzodioxin-5,8-dione, D-80174
5,7-Dihydroxy-1(3*H*)-isobenzofuranone, D-60339
2-Hydroxy-4,5-methylenedioxybenzaldehyde, H-70175

$C_8H_6O_5$
2-Formyl-3,4-dihydroxybenzoic acid, F-60070
2-Formyl-3,5-dihydroxybenzoic acid, F-60071
4-Formyl-2,5-dihydroxybenzoic acid, F-60072
6-Formyl-2,3-dihydroxybenzoic acid, F-60073
2-Hydroxy-1,3-benzenedicarboxylic acid, H-60101
2-Hydroxy-1,4-benzenedicarboxylic acid, H-70105
2-Hydroxy-3,4-methylenedioxybenzoic acid, H-60177
2-Hydroxy-4,5-methylenedioxybenzoic acid, H-80202
3-Hydroxy-4,5-methylenedioxybenzoic acid, H-60178
4-Hydroxy-2,3-methylenedioxybenzoic acid, H-60179
6-Hydroxy-2,3-methylenedioxybenzoic acid, H-60180
2,6,9-Trioxabicyclo[3.3.1]nona-3,7-diene-4,8-dicarboxaldehyde, T-80355

$C_8H_6O_6$
4,5-Dihydroxy-1,3-benzenedicarboxylic acid, D-60307

C_8H_6S
Cyclopenta[*b*]thiapyran, C-60224

$C_8H_6S_2$
2-(2,4-Cyclopentadienylidene)-1,3-dithiole, C-60221

$C_8H_7BF_4OS$
2-Methyl-1,3-benzoxathiazolium(1+); Tetrafluoroborate, *in* M-80053

$C_8H_7BrClNO_3$
5-Bromo-7-chlorocavernicolin, B-70199

C_8H_7BrO
2-Bromo-3-methylbenzaldehyde, B-60292

$C_8H_7BrO_2$
5′-Bromo-2′-hydroxyacetophenone, B-60265
Bromomethanol; Benzoyl, *in* B-80212
2-Bromo-3-methylbenzoic acid, B-60293
3-Bromo-4-methylbenzoic acid, B-60294

$C_8H_7BrO_2S$
2-Bromo-4-(methylthio)benzoic acid, *in* B-70226
2-Bromo-5-(methylthio)benzoic acid, *in* B-70227
3-Bromo-4-(methylthio)benzoic acid, *in* B-70228

$C_8H_7BrO_4$
4-Acetoxy-2-bromo-5,6-epoxy-2-cyclohexen-1-one, *in* B-60239

$C_8H_7Br_2F$
1,2-Bis(bromomethyl)-3-fluorobenzene, B-70131
1,2-Bis(bromomethyl)-4-fluorobenzene, B-70132
1,3-Bis(bromomethyl)-2-fluorobenzene, B-70133

$C_8H_7Br_2NO_2$
1,3-Bis(bromomethyl)-5-nitrobenzene, B-60145

$C_8H_7Br_2NO_3$
3,5-Dibromo-1,6-dihydroxy-4-oxo-2-cyclohexene-1-acetonitrile, D-60098

$C_8H_7ClN_4$
5-Chlorotetrazole; 1-Benzyl, *in* C-80113

$C_8H_7ClO_2$
▷ Benzyloxycarbonyl chloride, B-60071
Chloromethanol; Benzoyl, *in* C-80070
3-Chloro-4-methoxybenzaldehyde, *in* C-60089
4-Chloro-3-methoxybenzaldehyde, *in* C-60090

$C_8H_7ClO_2S$
5-Chloro-2-(methylthio)benzoic acid, *in* C-70085

$C_8H_7ClO_3$
3-Chloro-2,6-dihydroxy-4-methylbenzaldehyde, C-60059
3-Chloro-4,6-dihydroxy-2-methylbenzaldehyde, C-60060
3-Chloro-4-hydroxybenzoic acid; Me ester, *in* C-60091
3-Chloro-6-hydroxy-2-methoxybenzaldehyde, *in* C-60058
5-Chloro-2-hydroxy-3-methoxybenzaldehyde, *in* C-70065
2-Chloro-3-hydroxy-5-methylbenzoic acid, C-60095
3-Chloro-4-hydroxy-5-methylbenzoic acid, C-60096
5-Chloro-4-hydroxy-2-methylbenzoic acid, C-60097
3-Chloro-4-methoxybenzoic acid, *in* C-60091
3-Chloro-5-methoxybenzoic acid, *in* C-60092
4-Chloro-3-methoxybenzoic acid, *in* C-60093

$C_8H_7FN_4$
5-Fluoro-1*H*-tetrazole; 1-Benzyl, *in* F-80069

C_8H_7FO
2-Fluoro-2-phenylacetaldehyde, F-60062

$C_8H_7FO_2S$
4-Fluoro-2-mercaptobenzoic acid; Me ester, *in* F-70031

$C_8H_7FO_3$
3-Fluoro-2-hydroxybenzoic acid; Me ester, *in* F-60040
3-Fluoro-4-hydroxybenzoic acid; Me ester, *in* F-60041
4-Fluoro-2-hydroxybenzoic acid; Me ester, *in* F-60042
5-Fluoro-2-hydroxybenzoic acid; Me ester, *in* F-60044
2-Fluoro-5-methoxybenzoic acid, *in* F-60038
3-Fluoro-4-methoxybenzoic acid, *in* F-60041
5-Fluoro-2-methoxybenzoic acid, *in* F-60044

$C_8H_7F_3S$
1-(Methylthio)-4-(trifluoromethyl)benzene, *in* T-60286
2-(Trifluoromethyl)benzenemethanethiol, T-80278
3-(Trifluoromethyl)benzenemethanethiol, T-80279
4-(Trifluoromethyl)benzenemethanethiol, T-80280

C_8H_7IO
2-Iodoacetophenone, I-60039

$C_8H_7IO_2$
Iodomethanol; Benzoyl, *in* I-80033
5-Iodo-2-methoxybenzaldehyde, *in* H-70143

$C_8H_7IO_2S$
3-Iodo-4-(methylthio)benzoic acid, *in* I-70046

$C_8H_7IO_3$
2-Iodosophenylacetic acid, I-60063
1-Methoxy-1,2-benziodoxol-3(1*H*)one, *in* H-60102

C_8H_7N
Cyanocyclooctatetraene, *in* C-70239
Indolizine, I-60033
Isoindole, I-80063

C_8H_7NO
6-Hydroxyindole, H-60158
1(3*H*)-Isobenzofuranimine, I-70062
(Isocyanatomethyl)benzene, I-80055
2-Methylfuro[2,3-*b*]pyridine, M-60084
3-Methylfuro[2,3-*b*]pyridine, M-60085
Phthalimidine, P-70100

C_8H_7NOS
2*H*-1,4-Benzothiazin-3(4*H*)-one, B-80043

$C_8H_7NO_2$
5,6-Dihydroxyindole, D-70307

$C_8H_7NO_2S$
1-Nitro-2-(phenylthio)ethylene, N-70061

$C_8H_7NO_2S_2$
2*H*-1,4-Benzothiazine-3(4*H*)-thione; 1,1-Dioxide, *in* B-70055

$C_8H_7NO_3$
Amino-1,4-benzoquinone; *N*-Ac, *in* A-60089
2-Methyl-4-nitrobenzaldehyde, M-70096
(2-Nitrophenyl)oxirane, N-70056
(3-Nitrophenyl)oxirane, N-70057

$C_8H_7NO_3S$
1-Nitro-2-(phenylsulfinyl)ethylene, *in* N-70061

$C_8H_7NO_4$
2,4-Dihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, *in* D-10388
2-Hydroxy-4,5-methylenedioxybenzoic acid; Amide, *in* H-80202
2-Hydroxy-5-methyl-3-nitrobenzaldehyde, H-70180
4-(2-Nitroethenyl)-1,2-benzenediol, N-70049

$C_8H_7NO_4S$
1-Nitro-2-(phenylsulfonyl)ethylene, *in* N-70061

$C_8H_7NO_5$
3-Amino-4-hydroxy-1,2-benzenedicarboxylic acid, A-70151
4-Amino-5-hydroxy-1,2-benzenedicarboxylic acid, A-70152
4-Amino-6-hydroxy-1,3-benzenedicarboxylic acid, A-70153
5-Amino-2-hydroxy-1,3-benzenedicarboxylic acid, A-70154
5-Amino-4-hydroxy-1,3-benzenedicarboxylic acid, A-70155
2′,3′-Dihydroxy-6′-nitroacetophenone, D-60357
2′,5′-Dihydroxy-4′-nitroacetophenone, D-70322
3′,6′-Dihydroxy-2′-nitroacetophenone, D-60358
4′,5′-Dihydroxy-2′-nitroacetophenone, D-60359

$C_8H_7NO_6$
4-Hydroxy-5-methoxy-2-nitrobenzoic acid, *in* D-60360
5-Hydroxy-4-methoxy-2-nitrobenzoic acid, *in* D-60360

C_8H_7NS
2*H*-1,4-Benzothiazine, B-70053

$C_8H_7NS_2$
2*H*-1,4-Benzothiazine-3(4*H*)-thione, B-70055

$C_8H_7N_3$
1-Aminophthalazine, A-70184
5-Aminophthalazine, A-70185
4-Methyl-1,2,3-benzotriazine, M-80052
2-(1*H*-Pyrazol-1-yl)pyridine, P-70158
2-(1*H*-Pyrazol-3-yl)pyridine, P-70159
3-(1*H*-Pyrazol-1-yl)pyridine, P-70160
3-(1*H*-Pyrazol-3-yl)pyridine, P-70161
4-(1*H*-Pyrazol-1-yl)pyridine, P-70162
4-(1*H*-Pyrazol-3-yl)pyridine, P-70163
4-(1*H*-Pyrazol-4-yl)pyridine, P-70164

$C_8H_7N_3O$
2′-Azidoacetophenone, A-60334
3′-Azidoacetophenone, A-60335
4′-Azidoacetophenone, A-60336
2-Azido-3-methylbenzaldehyde, A-80201
2-Azido-5-methylbenzaldehyde, A-80202
1*H*-Benzotriazole; *N*-Ac, *in* B-70068
1,2-Dihydro-5-phenyl-3*H*-1,2,4-triazol-3-one, D-80241
Furo[2,3-*b*]pyridine-3-carboxaldehyde; Hydrazone, *in* F-60094
4-Methyl-1,2,3-benzotriazine; 2-Oxide, *in* M-80052
4-Methyl-1,2,3-benzotriazine; 3-Oxide, *in* M-80052

$C_8H_7N_3O_2$
6-Amino-2,3-dihydro-1,4-phthalazinedione, A-70134

$C_8H_7N_3O_4$
2-Nitro-1,3-benzenedicarboxylic acid; Diamide, *in* N-80035

$C_8H_7N_3S$
1,2,3-Benzotriazine-4(3*H*)-thione; 3-*N*-Me, *in* B-60050
1,2,3-Benzotriazine-4(3*H*)-thione; *S*-Me, *in* B-60050
4-Mercapto-2-methyl-1,2,3-benzotriazinium hydroxide inner salt, *in* B-60050

$C_8H_7N_5O_2$
2-Amino-4(1*H*)-pteridinone; N^2-Ac, *in* A-60242

$C_8H_7N_5O_8$
2,3,4,6-Tetranitroaniline; *N*-Di-Me, *in* T-60159

$C_8H_7OS^{\oplus}$
2-Methyl-1,3-benzoxathiazolium(1+), M-80053

C_8H_8
1,2-Dihydropentalene, D-70240
1,4-Dihydropentalene, D-70241
1,5-Dihydropentalene, D-70242
1,6-Dihydropentalene, D-70243
1,6*a*-Dihydropentalene, D-70244
5,6-Dimethylene-1,3-cyclohexadiene, D-70410
4-Methylene-1,2,5,6-heptatetraene, M-70070
4-Octene-1,7-diyne, O-60028
Pentacyclo[5.1.0.0^{2,4}.0^{3,5}.0^{6,8}]octane, P-80020

$C_8H_8BrNO_2$
3-Amino-2-bromobenzoic acid; Me ester, *in* A-70097

$C_8H_8BrNO_3$
2-Bromo-1-ethoxy-3-nitrobenzene, *in* B-70257

$C_8H_8Br_2O_4$
4-Acetoxy-2,6-dibromo-5-hydroxy-2-cyclohexen-1-one, *in* D-60097
2,6-Dibromo-4,5-dihydroxy-2-cyclohexen-1-one; 4-Ac, *in* D-60097

C_8H_8ClN
4-Chloro-2,3-dihydro-1*H*-indole, C-60055

$C_8H_8ClNO_3$
4-Chloro-2-ethoxy-1-nitrobenzene, *in* C-60119
1-Chloro-5-methoxy-2-methyl-3-nitrobenzene, *in* C-60116
2-Chloro-1-methoxy-3-methyl-4-nitrobenzene, *in* C-60115

$C_8H_8Cl_6O_4$
Hexahydro-2,5-bis(trichloromethyl)furo[3,2-*b*]furan-3*a*,6*a*-diol, H-70053

$C_8H_8FNO_2$
2-Amino-5-fluorobenzoic acid; Me ester, *in* A-70142
3-Amino-4-fluorobenzoic acid; Me ester, *in* A-70144
5-Amino-2-fluorobenzoic acid; Me ester, *in* A-70147

C_8H_8INO
2-Iodoacetophenone; Oxime (*Z*-), *in* I-60039

$C_8H_8INO_2$
3-Hydroxy-2-iodo-6-methylpyridine; *O*-Ac, *in* H-60159

$C_8H_8N_2$
1,1′-Dicyanobicyclopropyl, *in* B-70114
2-Methyl-1*H*-pyrrolo[2,3-*b*]pyridine, M-80156
2-Methyl-1*H*-pyrrolo[3,2-*b*]pyridine, M-80157
2-Methyl-1*H*-pyrrolo[2,3-*c*]pyridine, M-80158
2-Methyl-1*H*-pyrrolo[3,2-*c*]pyridine, M-80159
6*H*-Pyrrolo[3,4-*b*]pyridine; 6-Me, *in* P-70201
2*H*-Pyrrolo[3,4-*c*]pyridine; 2-Me, *in* P-70200

$C_8H_8N_2O$
▷ 1-(Diazomethyl)-4-methoxybenzene, D-60064
1,6-Dihydro-7*H*-pyrrolo[2,3-*c*]pyridin-7-one; 6-Me, *in* D-80252
3,4-Dihydro-2(1*H*)-quinazolinone, D-60278
Pyrrolo[1,2-*a*]pyrazin-1(2*H*)-one; *N*-Me, *in* P-70198

$C_8H_8N_2O_2$
Bicyclo[2.2.2]octa-5,7-diene-2,3-dione; Dioxime, *in* B-70109

$C_8H_8N_2O_2S$
Benzo[*b*]thiophen-3(2*H*)-one; Hydrazone, 1,1-dioxide, *in* B-60048

$C_8H_8N_2O_2S_2$
3-Mercapto-6(1*H*)-pyridazinethione; *S*,*S*-Di-Ac, *in* M-80028

$C_8H_8N_2O_3$
Nicotinuric acid, N-70034

$C_8H_8N_2O_4$
2-Hydroxy-5-methyl-3-nitrobenzaldehyde; Oxime, *in* H-70180
3,6-Pyridazinedicarboxylic acid; Di-Me ester, *in* P-70168

$C_8H_8N_2O_4S_2$
1,1′-Dithiobis-2,5-pyrrolidinedione, D-70524

$C_8H_8N_2O_6$
1,2-Dimethoxy-4,5-dinitrobenzene, *in* D-70449
1,5-Dimethoxy-2,4-dinitrobenzene, *in* D-80491
5-Ethoxy-2,4-dinitrophenol, *in* D-80491
Tartaric acid; Dinitrile, Di-Ac, *in* T-70005

$C_8H_8N_2S$
2-Amino-4*H*-3,1-benzothiazine, A-70092

$C_8H_8N_4$
2,4-Diaminoquinazoline, D-60048
▷ 1-Hydrazinophthalazine, H-60092

$C_8H_8N_4O$
2-Tetrazolin-5-one; 1-Benzyl, *in* T-60175

$C_8H_8N_4O_2$
2,4(1*H*,3*H*)-Pteridinedione; 1,3-Di-Me, *in* P-60191

$C_8H_8N_4O_3$
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione; 1,3-Di-Me, *in* P-70134
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione; 1,7-Di-Me, *in* P-70134
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione; 3,7-Di-Me, *in* P-70134
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1,3-Di-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1,6-Di-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1,8-Di-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 3,6-Di-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 3,8-Di-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 6,8-Di-Me, *in* P-70135

$C_8H_8N_4O_6$
2,4,6-Trinitroaniline; *N*-Di-Me, *in* T-70301

$C_8H_8N_4S$
1*H*-Tetrazole-5-thiol; 1-*N*-Ph, *S*-Me, *in* T-60174
Tetrazole-5-thione; 1-Me, 4-Ph, *in* T-60174

C_8H_8O
▷ Acetophenone, A-60017
Bicyclo[2.2.1]hepta-2,5-diene-2-carboxaldehyde, B-60083
Bicyclo[5.1.0]octa-3,5-dien-2-one, B-70111
4,7-Dihydroisobenzofuran, D-60253
▷ (4-Hydroxyphenyl)ethylene, H-70209
9-Oxabicyclo[4.2.1]nona-2,4,7-triene, O-70057
1-Phenylethenol, P-60092

C_8H_8OS
Benzeneethanethioic acid, B-70017
4′-Mercaptoacetophenone, M-60017
2-(Methylthio)benzaldehyde, *in* M-80018
4-(Methylthio)benzaldehyde, *in* M-80020
(Phenylthio)acetaldehyde, P-80136

$C_8H_8OS_3$
1,5-Dihydro-2,3,4-benzotrithiepin; 2-Oxide, *in* D-80176

$C_8H_8O_2$
Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid, B-60084
Bicyclo[2.2.2]oct-7-ene-2,5-dione, B-80086
Bicyclo[4.2.0]oct-7-ene-2,5-dione, B-60097
2-Hydroxy-4-methylbenzaldehyde, H-70160
2-(Hydroxymethyl)benzaldehyde, H-60171
3-Hydroxy-5-methylbenzaldehyde, H-80195
4-Hydroxy-2-methylbenzaldehyde, H-70161
2-Hydroxy-2-phenylacetaldehyde, H-60210
2-Hydroxyphenylacetaldehyde, H-60207
3-Hydroxyphenylacetaldehyde, H-60208
4-Hydroxyphenylacetaldehyde, H-60209
4-Vinyl-1,3-benzenediol, V-70010

$C_8H_8O_2S$
2-Mercapto-2-phenylacetic acid, M-60024

$C_8H_8O_3$
2,4-Dihydroxyphenylacetaldehyde, D-60369
2,5-Dihydroxyphenylacetaldehyde, D-60370
3,4-Dihydroxyphenylacetaldehyde, D-60371
7,10-Dioxaspiro[5.4]deca-2,5-dien-4-one, *in* B-70044
▷ 2-Hydroxy-3-methoxybenzaldehyde, *in* D-70285
3-Hydroxy-2-methoxybenzaldehyde, *in* D-70285
2-Hydroxy-4-methylbenzoic acid, H-70163
4-Hydroxy-2-methylbenzoic acid, H-70164

$C_8H_8O_4$
4,5-Dihydroxy-2-methylbenzoic acid, D-80339
3,6-Dimethoxy-1,2-benzoquinone, *in* D-60309
2-Hydroxy-3-methoxy-5-methyl-1,4-benzoquinone, *in* D-70320
3-Hydroxy-2-methoxy-5-methyl-1,4-benzoquinone, *in* D-70320
(2-Hydroxyphenoxy)acetic acid, H-70203
(3-Hydroxyphenoxy)acetic acid, H-70204
(4-Hydroxyphenoxy)acetic acid, H-70205
2′,4′,6′-Trihydroxyacetophenone, T-70248
▷ 3′,4′,5′-Trihydroxyacetophenone, T-60315

$C_8H_8O_5$
4,5-Dimethyl-2,3-furandicarboxylic acid, D-80449
3-Hydroxy-4-methoxy-1-methyl-7-oxabicyclo[4.1.0]hept-3-ene-2,5-dione, *in* D-70320
2,3,5-Trihydroxybenzoic acid; Me ester, *in* T-70250
3,4,6-Trihydroxy-2-methylbenzoic acid, T-80324
2,3,4-Trihydroxyphenylacetic acid, T-60340
2,3,5-Trihydroxyphenylacetic acid, T-60341
2,4,5-Trihydroxyphenylacetic acid, T-60342
3,4,5-Trihydroxyphenylacetic acid, T-60343

$C_8H_8O_6$
2,3-Diacetyl-2-butenedioic acid, D-80042

$C_8H_8O_7$
3,4-Diacetoxy-3,4-dihydro-2,5(2*H*,5*H*)-furandione, *in* T-70005

$C_8H_8S_2$
2-(2,4-Cyclopentadien-1-ylidene)-1,3-dithiolane, *in* C-60221
1,4- Dihydro-2,3-benzodithiin, D-80175

$C_8H_8S_3$
1,5-Dihydro-2,3,4-benzotrithiepin, D-80176

$C_8H_9BrO_3$
3-Bromo-2,6-dimethoxyphenol, *in* B-60200

$C_8H_9BrO_3S$
Bromomethanol; 4-Methylbenzenesulfonyl, *in* B-80212

$C_8H_9BrO_5$
(3-Bromo-2-oxopropylidene)propanedioic acid; Di-Me ester, *in* B-70262

C_8H_9ClO
1-(Chloromethyl)-2-methoxybenzene, *in* C-70101
1-(Chloromethyl)-3-methoxybenzene, *in* C-70102
1-Chloromethyl-4-methoxybenzene, *in* C-70103
2-Chloro-1-phenylethanol, C-80099
2-Chloro-2-phenylethanol, C-60128

$C_8H_9ClO_3S$
Chloromethanol; 4-Methylbenzenesulfonyl, *in* C-80070

C_8H_9F
2-Fluoro-1,3-dimethylbenzene, F-60026
1-Fluoro-2-phenylethane, F-80059

C_8H_9FO
1-Fluoro-2-methoxy-4-methylbenzene, *in* F-60054
1-Fluoro-3-methoxy-6-methylbenzene, *in* F-60057
1-Fluoro-4-methoxy-3-methylbenzene, *in* F-60059
2-Fluoro-1-methoxy-4-methylbenzene, *in* F-60053

$C_8H_9FO_2$
1-Fluoro-2,4-dimethoxybenzene, *in* F-70018
4-Fluoro-1,2-dimethoxybenzene, *in* F-60020

$C_8H_9IO_3S$
Iodomethanol; 4-Methylbenzenesulfonyl, *in* I-80033

C_8H_9N
N-Benzylidenemethylamine, B-60070
2-Cyanobicyclo[2.2.1]hepta-2,5-diene, *in* B-60084
6,7-Dihydro-5*H*-1-pyrindine, D-60275
6,7-Dihydro-5*H*-2-pyrindine, D-60276
3-(1-Propenyl)pyridine, P-80181

C_8H_9NO
Acetophenone; (*E*)-Oxime, *in* A-60017
2,3-Dihydro-5(1*H*)-indolizinone, D-60251
3,4-Dihydro-2*H*-pyrano[2,3-*b*]pyridine, D-80244
6,7-Dihydro-5*H*-1-pyrindine; *N*-Oxide, *in* D-60275
N-Methylbenzenecarboximidic acid, M-60045
1-(2-Pyridinyl)-2-propanone, P-60229
1-(3-Pyridinyl)-2-propanone, P-60230
1-(4-Pyridinyl)-2-propanone, P-60231

C_8H_9NOS
(Phenylthio)acetaldehyde; Oxime, *in* P-80136

$C_8H_9NO_2$
2-Hydroxy-4-methylbenzaldehyde; Oxime, *in* H-70160
4-Hydroxy-2-methylbenzaldehyde; Oxime, *in* H-70161
4-Hydroxyphenylacetaldoxime, *in* H-60209
2-(Methoxyacetyl)pyridine, *in* H-70101
Phenylacetohydroxamic acid, P-70059
3*a*,4,7,7*a*-Tetrahydro-1*H*-isoindole-1,3(2*H*)-dione, T-80070

$C_8H_9NO_2S$
1-Nitro-2-(phenylthio)ethane, N-70060

$C_8H_9NO_3$
3-Acetoxy-2-methyl-4(1*H*)-pyridinone, *in* H-80214
C-Benzyloxycarbohydroxamic acid, B-70086
1,4-Dihydro-6-methyl-4-oxo-3-pyridinecarboxylic acid; 1-Me, *in* D-80224
2-Formyl-1*H*-pyrrole-3-carboxylic acid; Et ester, *in* F-80077
4-Formyl-1*H*-pyrrole-2-carboxylic acid; Et ester, *in* F-80078
5-Formyl-1*H*-pyrrole-2-carboxylic acid; Et ester, *in* F-80079
5-Formyl-1*H*-pyrrole-2-carboxylic acid; 1-Me, Me ester, *in* F-80079
(2-Hydroxyphenoxy)acetic acid; Amide, *in* H-70203
4-(2-Nitroethyl)phenol, N-70050
1*H*-Pyrrole-3-carboxaldehyde; *N*-Ethoxycarbonyl, *in* P-70182

$C_8H_9NO_3S$
4-Carboxy-3-thiopheneacetic acid; *N*-Methylacetamide, *in* C-60018
2,3-Dihydro-1*H*-indole-2-sulfonic acid, D-70221
1-Nitro-2-(phenylsulfinyl)ethane, *in* N-70060

$C_8H_9NO_4$
3-Methoxy-2-methyl-6-nitrophenol, *in* M-70097
1*H*-Pyrrole-3,4-dicarboxylic acid; Di-Me ester, *in* P-70183

$C_8H_9NO_5$
3-Hydroxy-1*H*-pyrrole-2,5-dicarboxylic acid; Me ether, 2-Me ester, *in* H-80252
1*H*-Pyrrole-3,4-dicarboxylic acid; 1-Hydroxy, Di-Me ether, *in* P-70183

C_8H_9NS
Phenylthiolacetamide, *in* B-70017

$C_8H_9N_3$
1*H*-Benzotriazole; 1-Et, *in* B-70068

$C_8H_9N_5$
5-Amino-2-benzyl-2*H*-tetrazole, *in* A-70202
1-(Phenylmethyl)-1*H*-tetrazol-5-amine, *in* A-70202
N-(Phenylmethyl)-1*H*-tetrazol-5-amine, *in* A-70202

$C_8H_9N_5O_2$
N-(2,9-Dihydro-1-methyl-2-oxo-1*H*-purin-6-yl)acetamide, *in* A-60144

C_8H_{10}
Bicyclo[4.1.1]octa-2,4-diene, B-60090
Bicyclo[4.2.0]octa-2,4-diene, B-80085
1,3,5-Cyclooctatriene, C-80188
1-Ethynylcyclohexene, E-70051
5-Methyl-5-vinyl-1,3-cyclopentadiene, M-70146
Tetracyclo[3.3.0.0^{2,8}.0^{3,6}]octane, T-80025
Tetracyclo[3.3.0.0^{2,8}.0^{4,6}]octane, T-70022
Tetracyclo[4.2.0.0^{2,5}.0^{3,8}]octane, T-70023
1,2,3,4-Tetrahydropentalene, T-70076
1,2,3,5-Tetrahydropentalene, T-70077
1,2,4,5-Tetrahydropentalene, T-70078
1,2,3,3*a*-Tetrahydropentalene, T-70075
1,2,4,6*a*-Tetrahydropentalene, T-70079
1,2,6,6*a*-Tetrahydropentalene, T-70080
1,3*a*,4,6*a*-Tetrahydropentalene, T-70081
1,3*a*,6,6*a*-Tetrahydropentalene, T-70082
Tricyclo[3.2.1.0^{2,7}]oct-3-ene, T-60267
Tricyclo[5.1.0.0^{2,8}]oct-3-ene, T-60268
Tricyclo[5.1.0.0^{2,8}]oct-4-ene, T-60269

$C_8H_{10}Br_2O_4$
4-Acetoxy-2,6-dibromo-1,5-dihydroxy-2-cyclohexen-1-one, *in* D-60097

$C_8H_{10}ClN$
2-Chloro-3,5,6-trimethylpyridine, C-80121
3-Chloro-2,4,6-trimethylpyridine, C-80122
4-Chloro-2,3,5-trimethylpyridine, C-80123

$C_8H_{10}ClNO$
4-Chloro-2,3,5-trimethylpyridine; N-Oxide, *in* C-80123

$C_8H_{10}F_2O_4$
Difluoromaleic acid; Di-Et ester, *in* D-80159

$C_8H_{10}F_4O_4$
Tetrafluorobutanedioic acid; Di-Et ester, *in* T-80049

$C_8H_{10}IN$
2-Iodo-4,5-dimethylaniline, I-70028
4-Iodo-2,3-dimethylaniline, I-70029
4-Iodo-2,5-dimethylaniline, I-70030
4-Iodo-3,5-dimethylaniline, I-70031

$C_8H_{10}N_2$
Acetophenone; Hydrazone, *in* A-60017
1,4-Dihydropyrrolo[3,2-*b*]pyrrole; 1,4-Di-Me, *in* D-30286

$C_8H_{10}N_2O$
Acetamidoxime; *N*-Ph, *in* A-60016
1-(3-Pyridinyl)-2-propanone; Oxime, *in* P-60230

$C_8H_{10}N_2OS$
3-Amino-4(1*H*)-pyridinethione; *N*-Ac,*S*-Me, *in* A-80140
5-Amino-2(1*H*)-pyridinethione; *N*-Ac, *S*-Me, *in* A-80141

$C_8H_{10}N_2O_2$
3-Amino-4(1*H*)-pyridinone; 1-Me, N^3-Ac, *in* A-60254

$C_8H_{10}N_2O_3$
5-Ethyl-2,4(1*H*,3*H*)-pyrimidinedione; 1-Ac, *in* E-60054
5-Methoxy-2-methyl-3-nitroaniline, *in* A-60222

$C_8H_{10}N_2O_3S$
Aminoiminomethanesulfonic acid; *N*-Benzyl, *in* A-60210

$C_8H_{10}N_2O_4$
3-(2-Aminoethylidene)-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, A-70139
1*H*-Pyrazole-4,5-dicarboxylic acid; 1-Me, Di-Me ester, *in* P-80199
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidineacetic acid; Et ester, *in* T-70060

$C_8H_{10}N_4$
4-Amino-1*H*-imidazo[4,5-*c*]pyridine; 4-*N*-Di-Me, *in* A-70161

$C_8H_{10}N_4O_2$
1*H*-Pyrazolo[3,4-*d*]pyrimidine-4,6(5*H*,7*H*)-dione; 1,5,7-Tri-Me, *in* P-60202
1*H*-Pyrazolo[3,4-*d*]pyrimidine-4,6(5*H*,7*H*)-dione; 2,5,7-Tri-Me, *in* P-60202

$C_8H_{10}N_4O_5$
5-Nitrohistidine; N^{α}-Ac, *in* N-60028

$C_8H_{10}O$
Bicyclo[3.2.1]oct-6-en-3-one, B-80087
Bicyclo[4.2.0]oct-2-en-7-one, B-80088
4,4-Dimethyl-2,5-cyclohexadien-1-one, D-80441
6,6-Dimethyl-2,4-cyclohexadien-1-one, D-80442
3,3*a*,6,6*a*-Tetrahydro-1(2*H*)-pentalenone, T-70083
4,5,6,6*a*-Tetrahydro-2(1*H*)-pentalenone, T-70084
Tricyclo[3.2.1.0^{2,4}]octan-8-one, T-80243

$C_8H_{10}OS$
2-Mercaptobenzenemethanol; *S*-Me, *in* M-80021
4-Mercaptobenzenemethanol; *S*-Me, *in* M-80023
3-Mercaptobenzenemethanol; S-Me, *in* M-80022
Methyl 4-methylphenyl sulfoxide, M-70094

$C_8H_{10}O_2$
Bicyclo[4.2.0]octane-2,5-dione, B-60093
5,5-Dimethyl-2-cyclohexene-1,4-dione, D-70392
4,4-Dimethyl-3-oxo-1-cyclopentene-1-carboxaldehyde, D-60432
3-Ethynyl-3-methyl-4-pentenoic acid, E-60059
▷ 4-Methoxybenzyl alcohol, *in* H-80114
4-(Methoxymethyl)phenol, *in* H-80114
3*a*,4,7,7*a*-Tetrahydro-1(3*H*)-isobenzofuranone, T-70072
5-Vinyl-1-cyclopentenecarboxylic acid, V-60010

$C_8H_{10}O_2S$
4-Methyl-2-thiophenecarboxaldehyde; Ethylene acetal, *in* M-70141
1-(3-Thienyl)ethanol; Ac, *in* T-80179

$C_8H_{10}O_3$
2-Carbomethoxy-2-cyclohexen-1-one, *in* O-80079
Halleridone, H-60004
4-Hydroxy-3-methoxybenzenemethanol, *in* D-80284
4-Oxo-1-cycloheptene-1-carboxylic acid, O-70082
5-Oxo-1-cyclohexene-1-carboxylic acid; Me ester, *in* O-80077
5-Oxo-2-cyclohexene-1-carboxylic acid; Me ester, *in* O-80078

$C_8H_{10}O_3S$
1-Phenylethanesulfonic acid, P-70068

$C_8H_{10}O_4$
Bicyclo[1.1.1]pentane-1,3-dicarboxylic acid; Mono-Me ester, *in* B-80090
[1,1′-Bicyclopropyl]-1,1′-dicarboxylic acid, B-70114
2,3-Dicarbomethoxy-1,3-butadiene, *in* D-70409
3,6-Dimethoxy-1,2-benzenediol, *in* B-60014
5,5-Dimethyl-2-hexynedioic acid, D-70415
3,4-Epoxy-5-hydroxy-1-cyclohexenecarboxylic acid; Me ester, *in* E-80030
4-Hydroxy-2,5-dimethyl-3(2*H*)-furanone; Ac, *in* H-60120
3-Methoxy-6-methyl-1,2,4-benzenetriol, *in* M-80050
5-Methoxy-3-methyl-1,2,4-benzenetriol, *in* M-80048
6-Methoxy-3-methyl-1,2,4-benzenetriol, *in* M-80049
6-Methoxy-5-methyl-1,2,4-benzenetriol, *in* M-80049

$C_8H_{10}O_5$
5-Acetyl-2,2-dimethyl-1,3-dioxane-4,6-dione, A-60029
Diallyl dicarbonate, *in* D-70111
(2-Oxopropylidene)propanedioic acid; Di-Me ester, *in* O-70100

$C_8H_{10}O_8$
2,3-Di-*O*-acetyltartaric acid, *in* T-70005

$C_8H_{10}S$
2-Phenylethanethiol, P-70069

$C_8H_{10}S_2$
2,5-Dimethyl-1,4-benzenedithiol, D-60406

$C_8H_{11}BrO_2$
2-Bromobicyclo[2.2.1]heptane-1-carboxylic acid, B-60210
7-Bromo-5-heptynoic acid; Me ester, *in* B-60261

$C_8H_{11}BrO_3$
(3-Bromomethyl)-2,4,10-trioxatricyclo[3.3.1.1^{3,7}]decane, B-60301

$C_8H_{11}ClO_4$
Diethyl chlorofumarate, *in* C-80043

$C_8H_{11}ClO_5$
2,3-Dihydroxybutanoic acid; Di-Ac, chloride, *in* D-60312

$C_8H_{11}Cl_2N$
2,2-Dichloro-7-octenoic acid; Nitrile, *in* D-80123

$C_8H_{11}N$
1-Cyanocycloheptene, *in* C-80178

$C_8H_{11}NO$
Hexahydroazirino[2,3,1-*hi*]indol-2(1*H*)-one, H-70046
1,3,3*a*,4,5,7*a*-Hexahydro-2*H*-indol-2-one, H-70060
2-Methylene-1-azabicyclo[2.2.2]octan-3-one, M-80074
1,5,6,8*a*-Tetrahydro-3(2*H*)-indolizinone, T-70071
5,6,7,8-Tetrahydro-2(3*H*)-indolizinone, T-80068

$C_8H_{11}NOS$
N,*S*-Dimethyl-*S*-phenylsulfoximine, *in* M-80148

$C_8H_{11}NO_2$
3-Amino-2-cyclohexen-1-one; *N*-Ac, *in* A-70125
2,3-Dimethoxyaniline, *in* A-70089
▷ 3,4-Dimethoxyaniline, *in* A-70090
5-Methyl-1*H*-pyrrole-3-carboxylic acid; Et ester, *in* M-60125

$C_8H_{11}NO_3$
2,5-Dimethyl-4-oxazolecarboxylic acid; Et ester, *in* D-80461
3-Hydroxy-1*H*-pyrrole-2-carboxylic acid; Me ether, Et ester, *in* H-80248
4-Hydroxy-1*H*-pyrrole-2-carboxylic acid; Me ether, Et ester, *in* H-80249
4-Hydroxy-1*H*-pyrrole-3-carboxylic acid; Me ether, Et ester, *in* H-80250
4-Oxoheptanedioic acid; Me ester, mononitrile, *in* O-60071
2,4,6-Trimethoxypyridine, *in* D-70341

$C_8H_{11}NO_4$
5-Oxo-2-pyrrolidinecarboxylic acid; Me ester, *N*-Ac, *in* O-70102
5-Oxo-2-pyrrolidinecarboxylic acid; Me ester, *N*-benzoyl, *in* O-70102

$C_8H_{11}N_3$
2-Amino-5-vinylpyrimidine; N^2,N^2-Di-Me, *in* A-60269

$C_8H_{11}N_3O_3$
α-Amino-1*H*-imidazole-2-propanoic acid; N^{α}-Ac, *in* A-60205
5-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Ac, Et ester, *in* A-70192
3-Amino-1*H*-pyrazole-4-carboxylic acid; Et ester, *N*(3)-Ac, *in* A-70187
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidineacetic acid; *N*-Ethylamide, *in* T-70060

C_8H_{12}
Bicyclobutylidene, B-70095
Bicyclo[4.1.1]oct-2-ene, B-60095
Bicyclo[4.1.1]oct-3-ene, B-60096
1,2-Bis(methylene)cyclohexane, B-60166
1,3-Bis(methylene)cyclohexane, B-60167
1,4-Bis(methylene)cyclohexane, B-60168
3,3-Dimethyl-1,4-cyclohexadiene, D-80440
2,5-Dimethyl-1,3,5-hexatriene, D-60424
1,2,3,4,5,6-Hexahydropentalene, H-70066
1,2,3,3*a*,4,5-Hexahydropentalene, H-70064
1,2,3,3*a*,4,6*a*-Hexahydropentalene, H-70065
3-Methyl-1-vinylcyclopentene, M-80189
1,2,4-Octatriene, O-80019
1,3,5-Octatriene, O-70022
2,4,6-Octatriene, O-70023
3-Octen-1-yne, O-70029
Tricyclo[3.1.1.1^{2,4}]octane, T-60265
Tricyclo[5.1.0.0^{2,8}]octane, T-60266
3-Vinylcyclohexene, V-60009

$C_8H_{12}Br_2$
1,4-Dibromobicyclo[2.2.2]octane, D-70086

$C_8H_{12}Br_2O_3$
2-Bromo-2-methylpropanoic acid; Anhydride, *in* B-80229

$C_8H_{12}Cl_2$
1,4-Dichlorobicyclo[2.2.2]octane, D-70115

$C_8H_{12}Cl_2N_2O_2$
4,5-Dichloro-1*H*-imidazole-2-carboxaldehyde; Di-Et acetal, *in* D-60134

$C_8H_{12}Cl_2O_2$
2,2-Dichloro-7-octenoic acid, D-80123

$C_8H_{12}I_2$
1,4-Diiodobicyclo[2.2.2]octane, D-80397

$C_8H_{12}N_2$
3,4,5,6-Tetramethylpyridazine, T-80150

$C_8H_{12}N_2O$
2-*tert*-Butyl-4(3*H*)-pyrimidinone, B-60349

$C_8H_{12}N_2O_2$
[1,1′-Bipyrrolidine]-2,2′-dione, B-70125
Cyclo(prolylalanyl), C-80194
▷ 1,3-Diazaspiro[4.5]decane-2,4-dione, D-60056
4,4-Dimethyl-6-nitro-5-hexenenitrile, *in* D-60429

3-Ethoxy-4,5,6,7-tetrahydroisoxazolo[4,5-*c*]pyridine, *in* T-60071
Hexahydropyridazino[1,2-*a*]pyridazine-1,4-dione, H-70070

$C_8H_{12}N_2S_2$
2,3-Bis(methylthio)-1,4-benzenediamine, *in* D-60030
2,3-Bis(methylthio)-1,4-benzenediamine, *in* D-70036
4,6-Diamino-1,3-benzenedithiol; Di-*S*-Me, *in* D-70037

$C_8H_{12}N_4O_3$
2′,3′-Dideoxy-5-azacytidine, *in* A-80149

$C_8H_{12}N_4O_4$
2′-Deoxy-5-azacytidine, D-70022

$C_8H_{12}O$
1-Acetylcyclohexene, A-70038
4-Acetylcyclohexene, A-70039
1-Acetyl-2-methylcyclopentene, A-60043
Bicyclo[3.2.1]octan-8-one, B-60094
3-*tert*-Butyl-2-cyclobuten-1-one, B-80283
2-Isopropyl-5-methylfuran, I-80083
3-Methoxy-1-vinylcyclopentene, *in* V-80008
9-Oxabicyclo[6.1.0]non-4-ene, O-70058
2-(2-Propenyl)cyclopentanone, P-80178
2,5,5-Trimethyl-2-cyclopenten-1-one, T-70281

$C_8H_{12}O_2$
Bicyclo[2.2.1]heptane-1-carboxylic acid, B-60085
Bicyclo[3.1.1]heptane-1-carboxylic acid, B-60086
1-Cycloheptenecarboxylic acid, C-80178
5,6-Dimethoxy-1,3-cyclohexadiene, D-60397
2,2-Dimethyl-1,3-cyclohexanedione, D-80443
1,6-Dioxacyclodeca-3,8-diene, D-70458
1,4-Dioxaspiro[4,5]dec-7-ene, *in* C-60211
2,4-Dioxatricyclo[3.3.1.1^{3,7}]decane, D-80503
6-Ethyl-2,3-dihydro-2-methyl-4*H*-pyran-4-one, E-50071
6-Heptynoic acid; Me ester, *in* H-80033
3,5-Hexadienoic acid; Et ester, *in* H-70038
Hexahydro-2(3*H*)-benzofuranone, H-70049
Hexahydro-1(3*H*)-isobenzofuranone, H-70061
1-Methoxy-3-cyclohexene-1-carboxaldehyde, *in* H-80146
2-(Methoxymethylene)cyclohexanone, *in* O-80074
5-Methyl-3,4-hexadienoic acid; Me ester, *in* M-70087
2,6-Octadienoic acid, O-80011
2-Octenedial, O-80021
4-Octenedial, O-70025
7-Octynoic acid, O-80024
▷ 3-Oxiranyl-7-oxabicyclo[4.1.0]heptane, O-80056
2,2,4,4-Tetramethyl-1,3-cyclobutanedione, T-80143

$C_8H_{12}O_3$
4-Cyclohexene-1,2-diol; Mono-Ac, *in* C-80182
4,4-Diethoxy-2-butynal, *in* B-60351
3,6-Dihydro-2*H*-pyran-2-carboxylic acid; Et ester, *in* D-80242
2-Ethoxycarbonylcyclopentanone, *in* O-70084
3-Formyl-2,2-dimethyl-1-cyclopropanecarboxylic acid; Me ester, *in* F-80074
7-Hydroxy-5-heptynoic acid; Me ester, *in* H-60150
3-Oxocyclopentaneacetic acid; Me ester, *in* O-70083
4-Oxo-2-hexenoic acid; Et ester, *in* O-80082

$C_8H_{12}O_4$
3-Butene-1,2-diol; Di-Ac, *in* B-70291
3-(1,1-Dimethylethoxy)dihydro-2,5-furandione, *in* D-80211

$C_8H_{12}O_4S_2$
(Dimercaptomethylene)propanedioic acid; Di-*S*-Me, di-Me ester, *in* D-60395

$C_8H_{12}O_5$
Hydroxymethylenepropanedioic acid; Di-Et ester, *in* H-80204

$C_8H_{12}O_6$
2,3-Dihydroxybutanoic acid; Di-Ac, *in* D-60312

$C_8H_{13}BF_4O_2$
3,4,4*a*,5,6,7-Hexahydro-2*H*-pyrano[2,3-*b*]pyrilium; Tetrafluoroborate, *in* H-60055

$C_8H_{13}Br$
1-Bromobicyclo[2.2.2]octane, B-70184
1-Bromobicyclo[2.2.2]octane, B-80180
5-Bromo-3,3-dimethylcyclohexene, B-80199
1-Bromo-5-isopropylcyclopentene, B-80210

$C_8H_{13}Br_2NO_3$
6-Amino-2,2-dibromohexanoic acid; *N*-Ac, *in* A-60124

$C_8H_{13}Cl$
1-Chlorobicyclo[2.2.2]octane, C-70057

$C_8H_{13}Cl_2NO$
2,2-Dichloro-7-octenoic acid; Amide, *in* D-80123

$C_8H_{13}Cl_2NO_3$
6-Amino-2,2-dichlorohexanoic acid; *N*-Ac, *in* A-60126

$C_8H_{13}F$
1-Fluorobicyclo[2.2.2]octane, F-80028
2-Fluorobicyclo[3.2.1]octane, F-80029

$C_8H_{13}FO_2$
1-Fluorocyclohexanecarboxylic acid; Me ester, *in* F-80031

$C_8H_{13}I$
1-Iodobicyclo[2.2.2]octane, I-80019

$C_8H_{13}IO$
2-Iodocyclooctanone, I-70027

$C_8H_{13}NO$
1-Acetylcyclohexene; Oxime, *in* A-70038
3-Aminobicyclo[2.2.1]hept-5-ene-2-methanol, A-70094
1-Azabicyclo[3.3.1]nonan-2-one, A-70275
2-Azabicyclo[3.3.1]nonan-7-one, A-70276
Bicyclo[2.2.1]heptane-1-carboxylic acid; Amide, *in* B-60085
1-Cycloheptenecarboxylic acid; Amide, *in* C-80178

$C_8H_{13}NOS$
3,4-Dihydro-3,3,4,4-tetramethyl-5-thioxo-2(1*H*)pyrrolidinone, D-80255

$C_8H_{13}NO_2$
7-Aminobicyclo[4.1.0]heptane-7-carboxylic acid, A-60095
Hexahydro-2(3*H*)-benzoxazolone; *N*-Me, *in* H-70052
1-Hydroxy-3-cyclohexene-1-carboxaldehyde; Me ether, oxime, *in* H-80146
1-Oxa-2-azaspiro[2,5]octane; *N*-Ac, *in* O-70052

$C_8H_{13}NO_2S$
2-(Diethoxymethyl)thiazole, *in* T-80170

$C_8H_{13}NO_3$
4-Oxo-2-piperidinecarboxylic acid; *N*-Me, Me ester, *in* O-60089
3-Piperidinecarboxylic acid; *N*-Ac, *in* P-70102

$C_8H_{13}NO_4$
1-Amino-1,4-cyclohexanedicarboxylic acid, A-60117
2-Amino-1,4-cyclohexanedicarboxylic acid, A-60118
3-Amino-1,2-cyclohexanedicarboxylic acid, A-60119
4-Amino-1,1-cyclohexanedicarboxylic acid, A-60120
4-Amino-1,3-cyclohexanedicarboxylic acid, A-60121
3-Amino-2-oxetanone; *N*-*tert*-Butyloxycarbonyl, *in* A-80129
4,4-Dimethyl-6-nitro-5-hexenoic acid, D-60429

$C_8H_{13}NS_2$
3,3,4,4-Tetramethyl-2,5-pyrrolidinedithione, T-80151

$C_8H_{13}N_3O_2$
2-Azidocyclohexanol; Ac, *in* A-80196

$C_8H_{13}N_3O_2S$
Ovothiol *B*, *in* O-70050

$C_8H_{13}O_2^{\oplus}$
3,4,4*a*,5,6,7-Hexahydro-2*H*-pyrano[2,3-*b*]pyrilium, H-60055

$C_8H_{13}O_5P$
8,8*a*-Dihydro-3-methoxy-5-methyl-1*H*,6*H*-furo[3,4-*e*][1,3,2]dioxaphosphepin 3-oxide, D-70223

C_8H_{14}
Bicyclo[4.1.1]octane, B-60091
1-Ethylcyclohexene, E-60046
3-Ethylcyclohexene, E-70039
4-Ethylcyclohexene, E-60048
Methylenecycloheptane, M-80079

$C_8H_{14}BrNO_3$
6-Amino-2-bromohexanoic acid; *N*-Ac, *in* A-60100

$C_8H_{14}ClNO_3$
6-Amino-2-chlorohexanoic acid; *N*-Ac, *in* A-60109

$C_8H_{14}ClNO_4$
2,3,5,6,7,8-Hexahydro-1*H*-indolizinium(1+); Perchlorate, *in* H-70059

$C_8H_{14}N^{\oplus}$
2,3,5,6,7,8-Hexahydro-1*H*-indolizinium(1+), H-70059

$C_8H_{14}N_2$
4,5-Dihydro-3,3,5,5-tetramethyl-4-methylene-3*H*-pyrazole, D-60283

$C_8H_{14}N_2O_2$
1,3-Diazetidine-2,4-dione; 1,3-Diisopropyl, *in* D-60057
4,6-Diethoxy-2,5-dihydropyrimidine, *in* D-70256

$C_8H_{14}N_2O_4$
2,6-Diamino-4-methyleneheptanedioic acid, D-60039
2,2-Dimethyl-1,3-cyclohexanedione; Dioxime, *in* D-80443
2,5-Piperazinedicarboxylic acid; Di-Me ester, *in* P-60157
Proclavaminic acid, P-70116
N-Prolylserine, P-60173
N-Serylproline, S-60025

$C_8H_{14}N_2S_2$
4,6-Bis(ethylthio)-2,5-dihydropyrimidine, *in* D-70257

$C_8H_{14}N_4O_2$
Tetrahydroimidazo[4,5-*d*]imidazole-2,5(1*H*,3*H*)-dione; 1,3,4,6-Tetra-Me, *in* T-70066

$C_8H_{14}N_4S_2$
1,6-Diallyl-2,5-dithiobiurea, D-60026

$C_8H_{14}O$
2,2-Dimethyl-4-hexen-3-one, D-70414
2,2-Dimethyl-5-hexen-3-one, D-60425
3-Methyl-4-hepten-2-one, M-80093
4-Methyl-3-hepten-2-one, M-60087
6-Methyl-6-hepten-2-one, M-80094
2,4-Octadien-1-ol, O-70007
3-Octenal, O-70024
3-Octen-2-one, O-70027
4-Octen-2-one, O-60030
5-Octen-2-one, O-70028
2,2,3,3-Tetramethylcyclopropanecarboxaldehyde, T-70133
3,4,4-Trimethyl-1-pentyn-3-ol, T-80354

$C_8H_{14}OS$
Dihydro-3,3,4,4-tetramethyl-2(3*H*)-furanthione, D-60282
4,5-Dihydro-3,3,4,4-tetramethyl-2(3*H*)-thiophenone, D-60288
2,3,4,5,8,9-Hexahydrothionin; 1-Oxide, *in* H-70076

$C_8H_{14}O_2$
3,6-Dimethoxycyclohexene, *in* C-80181
4,4-Dimethoxycyclohexene, *in* C-60211
1,6-Dioxaspiro[4,5]decane, D-80501
4-Hexen-3-ol; Ac, *in* H-60077
3-Methyl-2-heptenoic acid, M-60086
4-Methyl-2-hexenoic acid; Me ester, *in* M-80101
2-Methyl-4-penten-1-ol; Ac, *in* M-80135
5-Octenoic acid, O-80022
4-Oxooctanal, O-60081
2,2,3,3-Tetramethylcyclopropanecarboxylic acid, T-80144

$C_8H_{14}O_2S$
S-Butyl 3-oxobutanethioate, *in* O-70080
S-*tert*-Butyl 3-oxobutanethioate, *in* O-70080
1,4-Dioxaspiro[4.5]decane-7-thiol, *in* M-70026
4-Mercapto-2-butenoic acid; *tert*-Butyl ester, *in* M-60018
Octahydrobenzo[*b*]thiophene; 1,1-Dioxide, *in* O-60012

$C_8H_{14}O_2S_2$
Bis(3-hydroxycyclobutyl)disulfide, *in* M-60019

$C_8H_{14}O_3$
2-Cyclohexyl-2-hydroxyacetic acid, C-60212
4,4-Dimethyl-5-oxopentanoic acid; Me ester, *in* D-60434
2-Formylpropanoic acid; *tert*-Butyl ester, *in* F-70039
2-Hydroxycyclohexanecarboxylic acid; Me ester, *in* H-70119
4-Hydroxy-4-(2-hydroxyethyl)cyclohexanone, H-60153
6-Methyl-5-oxoheptanoic acid, M-80130

$C_8H_{14}O_4$
(1-Methylpropyl)butanedioic acid, M-80150
L-Threaric acid; Mono-*tert-butyl ether*, *in* T-70005
L-Threaric acid; Mono-*tert*-butyl ester, *in* T-70005

$C_8H_{14}O_5$
3,3′-Oxybispropanoic acid; Di-Me ester, *in* O-80098

$C_8H_{14}O_6$
Diethyl tartrate, *in* T-70005

$C_8H_{14}S$
2,3,4,5,8,9-Hexahydrothionin, H-70076
Octahydrobenzo[*b*]thiophene, O-60012

$C_8H_{14}S_2$
4,5-Dihydro-3,3,4,4-tetramethyl-2(3*H*)-thiophenethione, D-60287

$C_8H_{15}Br$
1-Bromo-1-octene, B-70261

$C_8H_{15}BrO_2$
5-Bromo-2-hexanone; Ethylene acetal, *in* B-60262

$C_8H_{15}ClO$
2,2-Diethylbutanoic acid; Chloride, *in* D-60171
3,4,4-Trimethylpentanoic acid; Chloride, *in* T-80353

$C_8H_{15}F$
1-Fluoro-1-octene, F-70034

$C_8H_{15}I$
1-Iodo-1-octene, I-70051

$C_8H_{15}IO$
3-Iodo-2-octanone, I-60053

$C_8H_{15}N$
1-Azabicyclo[3.2.2]nonane, A-80190
1-Azabicyclo[3.3.1]nonane, A-80191
8-Azabicyclo[5.2.0]nonane, A-70274
1,2,3,6-Tetrahydropyridine; 1-Propyl, *in* T-70089
Tropane, *in* A-70278

$C_8H_{15}NO$
3-Aminobicyclo[2.2.1]heptane-2-methanol, A-70093
Hexahydro-5(2*H*)-azocinone; 1-Me, *in* H-70048
Octahydro-2*H*-1,3-benzoxazine, O-70011
Octahydro-2*H*-3,1-benzoxazine, O-70012
▷ Physoperuvine, P-60151
Tetrahydro-2-(2-pyrrolidinyl)furan, T-60090

$C_8H_{15}NO_2$
2-Aminocycloheptanecarboxylic acid, A-70123
3-Amino-2-hexenoic acid; Et ester, *in* A-60170
4,4-Diethoxybutanenitrile, *in* O-80068
2-Methyl-2-piperidinecarboxylic acid; Me ester, *in* M-60119
3-Piperidinecarboxylic acid; Et ester, *in* P-70102
4-(Tetrahydro-2-furanyl)morpholine, T-60065

$C_8H_{15}NO_3$
2-Amino-4,4-dimethylpentanoic acid; *N*-Formyl, *in* A-70137

$C_8H_{15}NO_4$
2-Amino-3-butylbutanedioic acid, A-60102

$C_8H_{15}N_5$
2,4,6-Triaminopyrimidine; N^4,N^6-Di-Et, *in* T-80208
2,4,6-Triaminopyrimidine; N^2,N^2,N^4,N^4-Tetra-Me, *in* T-80208
2,4,6-Triaminopyrimidine; N^4,N^4,N^6,N^6-Tetra-Me, *in* T-80208

C_8H_{16}
Isopropylcyclopentane, I-70092

$C_8H_{16}BrNO_2$
2-Amino-4-bromobutanoic acid; *tert*-Butyl ester, *in* A-60098

$C_8H_{16}Cl_2$
1,1-Dichlorooctane, D-70126
1,2-Dichlorooctane, D-70127
1,3-Dichlorooctane, D-70128
2,2-Dichlorooctane, D-70129
2,3-Dichlorooctane, D-70130
4,5-Dichlorooctane, D-70131

$C_8H_{16}N_2$
Decahydroquinazoline, D-70013
Octahydropyridazino[1,2-*a*]pyridazine, O-80016

$C_8H_{16}N_2O$
▷ Tetrahydro-2(1*H*)-pyrimidinone; 1,3-Di-Et, *in* T-60088

$C_8H_{16}N_2O_3S$
N-Methionylalanine, M-60035

$C_8H_{16}N_2O_4$
Octopinic acid, O-80023

$C_8H_{16}N_2O_4S$
N-Serylmethionine, S-60024

$C_8H_{16}N_4O_2$
1,3,5,7-Tetramethyltetrahydro-1,3,5,7-tetrazocine-2,6(1*H*,3*H*)dione, *in* T-70098

$C_8H_{16}O$
6-Methoxy-5-methyl-1-hexene, *in* M-80104
2-Octen-1-ol, O-60029
2,2,3,3-Tetramethylcyclopropanemethanol, T-70134

$C_8H_{16}OS$
2-Methyl-4-propyl-1,3-oxathiane, M-60122
3,3,4,4-Tetramethylthiolane; 1-Oxide, *in* T-80154

$C_8H_{16}OS_2$
4,4,5,5-Tetramethyl-1,2-dithiane; 1-Oxide, *in* T-80145

$C_8H_{16}O_2$
2,2-Diethylbutanoic acid, D-60171
2,5-Dimethoxy-3-hexene, *in* H-80083
3,4-Dimethylpentanoic acid; Me ester, *in* D-60435
4,4-Dimethylpentanoic acid; Me ester, *in* D-70428
5-Hydroxy-4-methyl-3-heptanone, H-60183
4-Octene-1,8-diol, O-70026
Pityol, P-60160
Tetrahydro-2,2,6-trimethyl-2*H*-pyran-3-ol, T-80081
3,4,4-Trimethylpentanoic acid, T-80353

$C_8H_{16}O_3$
1,1-Diethoxy-2-butanone, *in* O-80067
2-(Diethoxymethyl)oxetane, *in* O-80053
1-(2-Hydroxyethyl)-1,4-cyclohexanediol, H-60133
3-Hydroxy-3-methylpentanoic acid; Et ester, *in* H-80210
Isorengyol, *in* H-60133

$C_8H_{16}O_4$
Methyl 3,3-diethoxypropionate, *in* O-60090

$C_8H_{16}O_5$
5,7,8-Trimethoxyflavone, *in* T-60321

$C_8H_{16}O_6$
1,4-Di-*O*-methyl-*myo*-inositol, D-80452

$C_8H_{16}S$
3,3,4,4-Tetramethylthiolane, T-80154

$C_8H_{16}S_2$
1,1-Cyclohexanedimethanethiol, C-70223
1,2-Cyclohexanedimethanethiol, C-70224
1,2-Dithiecane, D-60507
4,4,5,5-Tetramethyl-1,2-dithiane, T-80145

$C_8H_{17}BrO$
8-Bromo-1-octanol, B-70260

$C_8H_{17}F$
1-Fluorooctane, F-80058

$C_8H_{17}N$
Octahydroazocine; 1-Me, *in* O-70010

$C_8H_{17}NO$
2-Aminocycloheptanemethanol, A-70124
2-(Aminomethyl)cycloheptanol, A-70168
2,2-Diethylbutanoic acid; Amide, *in* D-60171

$C_8H_{17}NO_3$
Levocarnitine; Me ether, *in* C-70024

$C_8H_{17}N_3O_3$
N-Ornithyl-β-alanine, O-60041

$C_8H_{18}N_2$
Hexahydropyrimidine; 1,3-Di-Et, *in* H-60056

$C_8H_{18}N_2O_2$
1,7-Dioxa-4,10-diazacyclododecane, D-60465

$C_8H_{18}N_4$
2,4,6,8-Tetramethyl-2,4,6,8-tetraazabicyclo[3.3.0]octane, *in* O-70015

$C_8H_{18}O_2$
2,2,3,3-Tetramethyl-1,4-butanediol, T-80141

$C_8H_{18}S_2$
2,2,3,3-Tetramethyl-1,4-butanedithiol, T-80142

$C_8H_{19}N$
2-Octylamine, O-60031

$C_8H_{19}NO_2$
4,4-Diethoxybutylamine, *in* A-80064

$C_8H_{19}N_3$
1,4,7-Triazacycloundecane, T-60234
1,4,8-Triazacycloundecane, T-60235

$C_8H_{22}N_4$
1,2-Dihydrazinoethane; $N^{\alpha},N^{\alpha'},N^{\beta},N^{\beta},N^{\beta'},N^{\beta'}$-Hexa-Me, *in* D-60192

$C_8O_2S_6$
2,6-Dithioxobenzo[1,2-*d*:4,5-*d*′]bis[1,3]dithiole-4,8-dione, D-60512

$C_8O_4S_2$
2,7-Dithiatricyclo[6.2.0.0^{3,6}]deca-1(8),3(6)-diene-4,5,9,10-tetrone, D-60506

$C_9H_3Cl_2NO_2$
6,7-Dichloro-5,8-isoquinolinedione, D-60137
6,7-Dichloro-5,8-quinolinedione, D-60149

$C_9H_3Cl_2NO_3$
6,7-Dichloro-5,8-quinolinedione; *N*-Oxide, *in* D-60149

$C_9H_4N_4O_2$
Tetrazolo[1,5-*b*]quinoline-5,10-dione, T-70156

$C_9H_4N_4O_3$
Imidazo[4,5-*g*]quinazoline-4,8,9(3*H*,7*H*)-trione, I-60010

$C_9H_4N_6O_2$
▷ 2,2-Diazido-1,3-indanedione, D-70056

C_9H_4O
2-(2-Propenyl)cyclohexanone, P-80177

$C_9H_4O_4$
3,4-Methylenedioxybenzocyclobutene-1,2-dione, *in* D-80274

$C_9H_5BrF_2$
3-Bromo-3,3-difluoro-1-phenylpropyne, B-70203

$C_9H_5BrO_2$
3-Bromo-4*H*-1-benzopyran-4-one, B-70183

$C_9H_5Br_2N_3$
4,5-Dibromo-6-phenyl-1,2,3-triazine, D-80097

$C_9H_5Cl_2F_3N_2$
5,6-Dichloro-2-(trifluoromethyl)-1*H*-benzimidazole; *N*-Me, *in* D-60160

$C_9H_5Cl_2N$
6,7-Dichloroisoquinoline, D-60136

$C_9H_5NO_2$
3-(Furo[3,4-*b*]furan-4-yl)-2-propenenitrile, F-70055
▷ 5,8-Isoquinolinequinone, I-60131

$C_9H_5NO_4$
6-Nitro-4*H*-1-benzopyran-4-one, N-80036

$C_9H_5NO_6$
4-Hydroxy-5-nitro-1,2-benzenedicarboxylic acid; Me ether, anhydride, *in* H-70191

$C_9H_5NS_2$
Dithieno[2,3-*b*:2′,3′-*d*]pyridine, D-70509
Dithieno[2,3-*b*:3′,2′-*d*]pyridine, D-70510
Dithieno[2,3-*b*:3′,4′-*d*]pyridine, D-70511
Dithieno[3,2-*b*:2′,3′-*d*]pyridine, D-70512
Dithieno[3,2-*b*:3′,4′-*d*]pyridine, D-70513
Dithieno[3,4-*b*:2′,3′-*d*]pyridine, D-70514
Dithieno[3,4-*b*:3′2′-*d*]pyridine, D-70515
Dithieno[3,4-*b*:3′,4′-*d*]pyridine, D-70516

C_9H_5NSe
2-Phenyl-1-(selenocyanato)acetylene, P-80134

$C_9H_5N_3O_2$
[1]-Benzopyrano[2,3-*d*]-1,2,3-triazol-9(1*H*)-one, B-60043

$C_9H_5N_3O_3$
2,3-Dicyano-1-methoxy-4-nitrobenzene, *in* H-70189

$C_9H_5N_3S$
2-Isothiocyanatoquinoxaline, I-80095

$C_9H_6BrN_3$
5-Bromo-4-phenyl-1,2,3-triazine, B-80252

C_9H_6ClNO
▷ 5-Chloro-8-hydroxyquinoline, C-70075
8-Chloro-2(1*H*)-quinolinone, C-60131
8-Chloro-4(1*H*)-quinolinone, C-60132
1*H*-Indole-3-acetic acid; Chloride, *in* I-70013

$C_9H_6ClNO_2$
5-Chloro-8-hydroxyquinoline; 1-Oxide, *in* C-70075
1-(Chloromethyl)-1*H*-indole-2,3-dione, C-70092

C_9H_6ClNS
2-Chloro-4-phenylthiazole, C-80107

$C_9H_6Cl_2O_2$
1,3,5-Cycloheptatriene-1,6-dicarboxylic acid; Dichloride, *in* C-60202

C_9H_6FN
2-Fluoroquinoline, F-80062
3-Fluoroquinoline, F-80063
4-Fluoroquinoline, F-80064
▷ 5-Fluoroquinoline, F-80065
▷ 6-Fluoroquinoline, F-80066
7-Fluoroquinoline, F-80067
▷ 8-Fluoroquinoline, F-80068

C_9H_6FNO
2-Fluoroquinoline; *N*-oxide, *in* F-80062
3-Fluoroquinoline; *N*-oxide, *in* F-80063
5-Fluoroquinoline; *N*-oxide, *in* F-80065
6-Fluoroquinoline; *N*-oxide, *in* F-80066
8-Fluoroquinoline; *N*-oxide, *in* F-80068

$C_9H_6F_2O$
2,3-Difluoro-3-phenyl-2-propenal, D-80164

$C_9H_6F_3N$
2-Trifluoromethyl-1*H*-indole, T-60291
3-Trifluoromethyl-1*H*-indole, T-60292
6-Trifluoromethyl-1*H*-indole, T-60293

$C_9H_6N_2$
3-Cyanoindole, *in* I-80012
Imidazo[5,1,2-*cd*]indolizine, I-70004

$C_9H_6N_2O$
3-Cinnolinecarboxaldehyde, C-70178
4-Cinnolinecarboxaldehyde, C-70179

$C_9H_6N_2O_2$
5,8-Isoquinolinequinone; 8-Oxime, *in* I-60131
1-Nitroisoquinoline, N-60029
4-Nitroisoquinoline, N-60030
5-Nitroisoquinoline, N-60031
6-Nitroisoquinoline, N-60032
7-Nitroisoquinoline, N-60033
8-Nitroisoquinoline, N-60034
5-Phenyl-1,2,4-oxadiazole-3-carboxaldehyde, P-60122

$C_9H_6N_2O_3$
2-Methyl-4,5,8-quinazolinetrione, M-80160
5-Nitroisoquinoline; 2-Oxide, *in* N-60031
8-Nitroisoquinoline; 2-Oxide, *in* N-60034

$C_9H_6N_2S$
3-Amino-2-cyanobenzo[*b*]thiophene, *in* A-60091

$C_9H_6N_4$
4-Cyano-2-phenyl-1,2,3-triazole, *in* P-60140
1*H*-1,2,3-Triazolo[4,5-*f*]quinoline, T-70207
1*H*-1,2,3-Triazolo[4,5-*h*]quinoline, T-70208

$C_9H_6N_4O$
1,5-Dihydro-8*H*-imidazo[4,5-*g*]quinazolin-8-one, I-60012
3,8-Dihydro-9*H*-pyrazolo[4,3-*f*]quinazolin-9-one, D-60271
Imidazo[4,5-*f*]quinazolin-9(8*H*)-one, I-60011
Imidazo[4,5-*h*]quinazolin-6-one, I-60013
Pyrazolo[3,4-*f*]quinazolin-9(8*H*)-one, P-60204
Pyrazolo[4,3-*g*]quinazolin-5(6*H*)-one, P-60205

$C_9H_6N_4O_2$
Imidazo[4,5-*g*]quinazoline-6,8(5*H*,7*H*)-dione, I-60009
1*H*-Pyrazolo[4,3-*g*]quinazoline-5,7(6*H*,8*H*)-dione, P-60203

$C_9H_6N_4S$
Pyrazino[2,3-*b*]pyrido[3′,2′-*e*][1,4]thiazine, P-60199

C_9H_6O
5*H*-Cyclopropa[*f*]isobenzofuran, C-70251
4-Ethynylbenzaldehyde, E-70048

C_9H_6OS
5-(2-Thienyl)-2-penten-4-ynal, T-80182

$C_9H_6O_2$
▷ 1*H*-2-Benzopyran-1-one, B-60041

$C_9H_6O_2S$
4-Hydroxy-2*H*-1-benzothiopyran-2-one, H-70110
5-(2-Thienyl)-2-penten-4-ynoic acid, T-80183

$C_9H_6O_3$
3-Benzofurancarboxylic acid, B-60032
6-Hydroxy-2*H*-1-benzopyran-2-one, H-70109
3-Methyl-4,5-benzofurandione, M-70051

$C_9H_6O_4$
6,7-Dihydroxy-2*H*-1-benzopyran-2-one, D-84287
4-Hydroxy-5-benzofurancarboxylic acid, H-60103
5-Hydroxy-3-methyl-1,2-benzenedicarboxylic acid; Anhydride, *in* H-70162

$C_9H_6O_5$
4,5,7-Trihydroxy-2H-1-benzopyran-2-one, T-80286
5,6,7-Trihydroxy-2*H*-1-benzopyran-2-one, T-80287
5,7,8-Trihydroxy-2*H*-1-benzopyran-2-one, T-80288

$C_9H_6O_{12}$
Cyclopropanehexacarboxylic acid, C-70250

C_9H_6S
5*H*-Cyclopropa[*f*][2]benzothiophene, C-70247

$C_9H_6S_6$
Benzo[1,2-*d*:3,4-*d*′:5,6-*d*″]tris[1,3]dithiole, B-70069

C_9H_7Br
3-Bromo-3-phenyl-1-propyne, B-80244

$C_9H_7BrN_2$
5-Bromo-1-phenylpyrazole, *in* B-80253
3(5)-Bromopyrazole; 1-Ph, *in* B-80253
4-Bromopyrazole; 1-Ph, *in* B-80254

$C_9H_7Br_3O$
3,5-Dimethyl-2,4,6-tribromobenzaldehyde, D-80476

$C_9H_7ClN_2$
1-Chloro-4-methylphthalazine, C-70104
2-Chloro-3-methylquinoxaline, C-70121
2-Chloro-5-methylquinoxaline, C-70122
2-Chloro-6-methylquinoxaline, C-70123
2-Chloro-7-methylquinoxaline, C-70124
2-(Chloromethyl)quinoxaline, C-70120
6-Chloro-7-methylquinoxaline, C-70125

$C_9H_7ClN_2O$
2-Chloro-3-methylquinoxaline; 1-Oxide, *in* C-70121
2-Chloro-3-methylquinoxaline; 4-Oxide, *in* C-70121
3-Chloro-7-methylquinoxaline 1-oxide, *in* C-70123
6-Chloro-7-methylquinoxaline; 1-Oxide, *in* C-70125

$C_9H_7ClN_2O_2$
2-Chloro-3-methylquinoxaline; 1,4-Dioxide, *in* C-70121
6-Chloro-7-methylquinoxaline; 1,4-Dioxide, *in* C-70125

$C_9H_7ClO_3$
1,4-Benzodioxan-2-carboxylic acid; Chloride, *in* B-60024
1,4-Benzodioxan-6-carboxylic acid; Chloride, *in* B-60025

$C_9H_7ClO_4$
2-Hydroxy-4,5-methylenedioxybenzoic acid; Me ether, chloride, *in* H-80202
3-Hydroxy-4,5-methylenedioxybenzoic acid; Me ether, chloride, *in* H-60178

$C_9H_7ClO_4S$
1-Benzothiopyrylium(1+); Perchlorate, *in* B-70066
2-Benzothiopyrylium(1+); Perchlorate, *in* B-70067

$C_9H_7Cl_3O$
3,5-Dimethyl-2,4,6-trichlorobenzaldehyde, D-80477

$C_9H_7F_3O_2$
4-Methoxy-2-(trifluoromethyl)benzaldehyde, *in* H-70228
4-Methoxy-3-(trifluoromethyl)benzaldehyde, *in* H-70229

$C_9H_7F_3S$
1-(Methylthio)-3-(trifluoromethyl)benzene, *in* T-60285

C_9H_7IO
2-Iodo-3-phenyl-2-propenal, I-80039

$C_9H_7IO_4$
1-Hydroxy-1,2-benziodoxol-3(1*H*)-one; Ac, *in* H-60102

C_9H_7N
Cyclopent[*b*]azepine, C-60225

C_9H_7NO
o-Cyanoacetophenone, *in* A-80015
Cyclohepta[*b*]pyrrol-2(1*H*)-one, C-60201
Cyclopent[*b*]azepine; *N*-Oxide, *in* C-60225
5,6-Epoxyquinoline, E-60027
7,8-Epoxyquinoline, E-60028
6-Hydroxyisoquinoline, H-80178
1*H*-Indole-5-carboxaldehyde, I-60029
1*H*-Indole-6-carboxaldehyde, I-60030
1*H*-Indole-7-carboxaldehyde, I-60031
5-Phenyloxazole, P-60125
3*H*-Pyrrolo[1,2-*a*]azepin-3-one, P-70190
5*H*-Pyrrolo[1,2-*a*]azepin-5-one, P-70191
7*H*-Pyrrolo[1,2-*a*]azepin-7-one, P-70192
9*H*-Pyrrolo[1,2-*a*]azepin-9-one, P-70193
2-Vinylbenzoxazole, V-80006

C_9H_7NOS
1,4-Benzothiazepin-5(4*H*)-one, B-80040

$C_9H_7NO_2$
1,4-Benzodioxan-2-carbonitrile, *in* B-60024
1,3-Benzodioxole-4-acetonitrile, *in* B-60029
2,3-Dihydro-1,4-isoquinolinedione, D-80217
1*H*-Indole-3-carboxylic acid, I-80012
1,3(2*H*,4*H*)-Isoquinolinedione, I-70099

$C_9H_7NO_2S$
▷ 3-Amino-2-benzo[*b*]thiophenecarboxylic acid, A-60091
2*H*-3,1-Benzothiazine-2,4(1*H*)-dione; *N*-Me, *in* B-80042

$C_9H_7NO_3$
1,5-Benzoxepine-2,4-(3*H*,5*H*)-dione, B-80053
3,5-Dihydroxy-4-phenylisoxazole, D-70337
1*H*-Isoindolin-1-one-3-carboxylic acid, I-60102
3-Methoxy-4,5-methylnedioxybenzonitrile, *in* H-60178

$C_9H_7NO_4$
3-Amino-4-hydroxy-1,2-benzenedicarboxylic acid; Me ether, anhydride, *in* A-70151
5,6-Dihydroxy-1*H*-indole-2-carboxylic acid, D-70308

$C_9H_7NO_6$
2-Nitro-1,3-benzenedicarboxylic acid; Mono-Me ester, *in* N-80035

$C_9H_7NO_7$
3-Methoxy-6-nitro-1,2-benzenedicarboxylic acid, *in* H-70189
4-Methoxy-3-nitro-1,2-benzenedicarboxylic acid, *in* H-70190
4-Methoxy-5-nitro-1,2-benzenedicarboxylic acid, *in* H-70191
4-Methoxy-5-nitro-1,3-benzenedicarboxylic acid, *in* H-70192

C_9H_7NS
1(2*H*)-Isoquinolinethione, I-60132
3(2*H*)-Isoquinolinethione, I-60133
3-Quinolinethiol, Q-60003
5-Quinolinethiol, Q-60004
6-Quinolinethiol, Q-60005
4(1*H*)-Quinolinethione, Q-60006

$C_9H_7NS_2$
4-Phenyl-2(3*H*)-thiazolethione, P-80135

$C_9H_7N_3O$
4-Benzoyl-1,2,3-triazole, B-70079
4-Cinnolinecarboxaldehyde; Oxime, *in* C-70179

$C_9H_7N_3OS$
1,2,3-Benzotriazine-4(3*H*)-thione; *N*-Ac, *in* B-60050

$C_9H_7N_3O_2$
6-Amino-8-nitroquinoline, A-60234
8-Amino-6-nitroquinoline, A-60235
5-Phenyl-1,2,4-oxadiazole-3-carboxaldehyde; Oxime, *in* P-60122
2-Phenyl-2*H*-1,2,3-triazole-4-carboxylic acid, P-60140

$C_9H_7N_5$
8-Aminoimidazo[4,5-*g*]quinazoline, A-60207

$C_9H_7N_5O$
7-Amino-1,6-dihydro-9*H*-imidazo[4,5-*f*]quinazolin-9-one, A-60208
6-Amino-1,7-dihydro-8*H*-imidazo[4,5-*g*]quinazolin-8-one, A-60209

$C_9H_7S^{\oplus}$
1-Benzothiopyrylium(1+), B-70066
2-Benzothiopyrylium(1+), B-70067

$C_9H_8ClNO_5$
4,5-Dihydroxy-2-nitrobenzoic acid; Di-Me ether, chloride, *in* D-60360

$C_9H_8Cl_3NO_2$
2-Amino-3-(2,3,4-trichlorophenyl)propanoic acid, A-60262
2-Amino-3-(2,3,6-trichlorophenyl)propanoic acid, A-60263
2-Amino-3-(2,4,5-trichlorophenyl)propanoic acid, A-60264

$C_9H_8FNO_3$
2-Amino-4-fluorobenzoic acid; *N*-Ac, *in* A-70141
2-Amino-5-fluorobenzoic acid; *N*-Ac, *in* A-70142
3-Amino-4-fluorobenzoic acid; *N*-Ac, *in* A-70144
4-Amino-2-fluorobenzoic acid; *N*-Ac, *in* A-70145
4-Amino-3-fluorobenzoic acid; *N*-Ac, *in* A-70146

$C_9H_8F_3NO$
3,3,3-Trifluoropropanoic acid; Anilide, *in* T-80284

$C_9H_8N_2$
1*H*-1,2-Benzodiazepine, B-80019
1*H*-Cyclooctapyrazole, C-70236

$C_9H_8N_2O$
5-Amino-3-phenylisoxazole, A-60240
3-Amino-2(1*H*)-quinolinone, A-60256
3*H*-1,2-Benzodiazepine; 1-Oxide, *in* B-80020
3*H*-1,2-Benzodiazepine; 2-Oxide, *in* B-80020
2,2′-Bi-1*H*-pyrrole-5-carboxaldehyde, B-80130
N-Hydroxy-4-quinolinamine, H-80253
5-Methyl-3-phenyl-1,2,4-oxadiazole, M-60110
1*H*-Pyrrolo[3,2-*b*]pyridine; *N*-Ac, *in* P-60249

$C_9H_8N_2OS$
3-Amino-2-benzo[*b*]thiophenecarboxylic acid; Amide, *in* A-60091
1,2,3,4-Tetrahydro-2-thioxo-5*H*-1,4-benzodiazepin-5-one, T-70100
▷ 2-Thioxo-4-imidazolidinone; 3-*N*-Ph, *in* T-70188

$C_9H_8N_2O_2$
1,4-Dihydro-2,3-quinoxalinedione; 1-Me, *in* D-60279
3,5-Dihydroxy-4-phenylpyrazole, D-80369
6-Hydroxy-7-methoxyquinoxaline, *in* Q-60009
N-Hydroxy-4-quinolinamine; 1-Oxide, *in* H-80253
3,5-Pyrazolidinedione; 1-Ph, *in* P-80200

$C_9H_8N_2O_3$
5-Phenyl-1,2,4-oxadiazole-3-carboxaldehyde; Covalent hydrate, *in* P-60122

$C_9H_8N_2O_4$
1-Cyano-4,5-dimethoxy-2-nitrobenzene, *in* D-60360

$C_9H_8N_2O_6$
3,5-Dinitrobenzoic acid; Et ester, *in* D-60458

$C_9H_8N_2O_7$
4,5-Dinitro-1,2-benzenediol; Mono-Me ether, Ac, *in* D-70449

$C_9H_8N_2S$
3-Amino-2(1*H*)quinolinethione, A-70197
4-Methyl-5-phenyl-1,2,3-thiadiazole, M-60116
5-Methyl-4-phenyl-1,2,3-thiadiazole, M-60117

$C_9H_8N_4$
4-Cinnolinecarboxaldehyde; Hydrazone, *in* C-70179

$C_9H_8N_4O$
2-Phenyl-2*H*-1,2,3-triazole-4-carboxylic acid; Amide, *in* P-60140

$C_9H_8N_6O_3$
Lepidopterin, L-60020

C_9H_8O
Bicyclo[4.2.1]nona-2,4,7-trien-9-one, B-80084
Cyclooctatetraenecarboxaldehyde, C-70238
3-Phenyl-2-propyn-1-ol, P-60130

C_9H_8OS
1,4-Dihydro-3*H*-2-benzothiopyran-3-one, D-60206

C_9H_8OSe
1*H*-2-Benzoselenin-4(3*H*)-one, B-70051
1,4-Dihydro-3*H*-2-benzoselenin-3-one, D-60204

C_9H_8OTe
1,4-Dihydro-3*H*-2-benzotellurin-3-one, D-60205

$C_9H_8O_2$
1*H*-2-Benzopyran-4(3*H*)-one, B-70042
Cubanecarboxylic acid, C-60174
Cyclooctatetraenecarboxylic acid, C-70239
1,4-Dihydro-2(3*H*)-benzopyran-3-one, D-70176
4-Hydroxybenzofuran, H-70106
3-(4-Hydroxyphenyl)-2-propenal, H-60213
4-Methoxybenzofuran, *in* H-70106
2-Methyl-1,3-benzenedicarboxaldehyde, M-60046
2-Methyl-1,4-benzenedicarboxaldehyde, M-60047
4-Methyl-1,2-benzenedicarboxaldehyde, M-60048
4-Methyl-1,3-benzenedicarboxaldehyde, M-60049
5-Methyl-1,3-benzenedicarboxaldehyde, M-60050

$C_9H_8O_2S$
2-Acetyl-3-hydroxy-5-(1-propynyl)thiophene, A-80024
3,4-Dihydro-2*H*-1,5-benzoxathiepin-3-one, D-60207
3-(2-Thienyl)-2-propenoic acid; Me ester, *in* T-60208

$C_9H_8O_3$
2-Acetylbenzoic acid, A-80015
5-Acetyl-2-hydroxybenzaldehyde, A-80022
1,4-Benzodioxan-2-carboxaldehyde, B-60022
1,4-Benzodioxan-6-carboxaldehyde, B-60023
4*H*-1,3-Benzodioxin-6-carboxaldehyde, B-60026
2,3-Dihydro-2-benzofurancarboxylic acid, D-60197
▷ 3-(4-Hydroxyphenyl)-2-propenoic acid, H-80242
2-Methoxy-3(2*H*)-benzofuranone, *in* H-80107
4-Methoxy-3(2*H*)-benzofuranone, *in* H-80108
5-Methoxy-3(2*H*)-benzofuranone, *in* H-80109
6-Methoxy-3(2*H*)-benzofuranone, *in* H-80110
7-Methoxy-3(2*H*)-benzofuranone, *in* H-80111

$C_9H_8O_4$
1,4-Benzodioxan-2-carboxylic acid, B-60024
1,4-Benzodioxan-6-carboxylic acid, B-60025
4*H*-1,3-Benzodioxin-6-carboxylic acid, B-60027
1,3-Benzodioxole-4-acetic acid, B-60029
1,3,5-Cycloheptatriene-1,6-dicarboxylic acid, C-60202
5,7-Dihydroxy-6-methyl-1(3*H*)-isobenzofuranone, D-60349
5-Hydroxy-7-methoxyphthalide, *in* D-60339
7-Hydroxy-5-methoxyphthalide, *in* D-60339

3-(4-Hydroxyphenyl)-2-oxopropanoic acid, H-80238
2-Methoxy-4,5-methylenedioxybenzaldehyde, *in* H-70175

$C_9H_8O_5$
2-Formyl-3,5-dihydroxybenzoic acid; Me ester, *in* F-60071
2-Hydroxy-1,3-benzenedicarboxylic acid; Mono-Me ester, *in* H-60101
5-Hydroxy-3-methyl-1,2-benzenedicarboxylic acid, H-70162
2-Methoxy-1,3-benzenedicarboxylic acid, *in* H-60101
2-Methoxy-1,4-benzenedicarboxylic acid, *in* H-70105
5-Methoxy-1,3-benzodioxole-4-carboxylic acid, *in* H-60180
6-Methoxy-1,3-benzodioxole-5-carboxylic acid, *in* H-80202
7-Methoxy-1,3-benzodioxole-4-carboxylic acid, *in* H-60179
2-Methoxy-3,4-methylenedioxybenzoic acid, *in* H-60177
3-Methoxy-4,5-methylenedioxybenzoic acid, *in* H-60178
3-Oxotricyclo[2.1.0.0^{2,5}]pentane-1,5-dicarboxylic acid; Di-Me ester, *in* O-80096

$C_9H_8O_7$
2-Oxo-1,3-cyclopentanediglyoxylic acid, O-70085

C_9H_9BrO
3-(Bromomethyl)-2,3-dihydrobenzofuran, B-60295
▷ 2-Bromo-1-phenyl-1-propanone, B-80243

$C_9H_9BrO_2$
1-(5-Bromo-2-methoxyphenyl)ethanone, *in* B-60265

$C_9H_9Br_3$
1,3,5-Tris(bromomethyl)benzene, T-60401

C_9H_9Cl
1-Chloro-2-(2-propenyl)benzene, C-70152
1-Chloro-3-(2-propenyl)benzene, C-70153
1-Chloro-4-(2-propenyl)benzene, C-70154

C_9H_9ClO
2-Chloro-4,6-dimethylbenzaldehyde, C-60061
4-Chloro-2,6-dimethylbenzaldehyde, C-60062
4-Chloro-3,5-dimethylbenzaldehyde, C-60063
5-Chloro-2,4-dimethylbenzaldehyde, C-60064

$C_9H_9ClO_2$
3-(Chloromethyl)phenol; Ac, *in* C-70102

$C_9H_9ClO_3$
5-Chloro-2,3-dimethoxybenzaldehyde, *in* C-70065
3-Chloro-4-hydroxybenzoic acid; Me ester, Me ether, *in* C-60091
2-Chloro-3-methoxy-5-methylbenzoic acid, *in* C-60095
3-Chloro-4-methoxy-5-methylbenzoic acid, *in* C-60096
5-Chloro-4-methoxy-2-methylbenzoic acid, *in* C-60097
4-(Chloromethyl)phenol; Ac, *in* C-70103

$C_9H_9Cl_2NO_2$
2-Amino-3-(2,3-dichlorophenyl)propanoic acid, A-60127
2-Amino-3-(2,4-dichlorophenyl)propanoic acid, A-60128
2-Amino-3-(2,5-dichlorophenyl)propanoic acid, A-60129
2-Amino-3-(2,6-dichlorophenyl)propanoic acid, A-60130
2-Amino-3-(3,4-dichlorophenyl)propanoic acid, A-60131
2-Amino-3-(3,5-dichlorophenyl)propanoic acid, A-60132

$C_9H_9Cl_3$
1,3,5-Tris(chloromethyl)benzene, T-60402

C_9H_9FO
2-Fluoro-2-phenylpropanal, F-60063
2-Fluoro-3-phenylpropanal, F-60064
2-Fluoro-1-phenyl-1-propanone, F-60065

$C_9H_9FO_2$
3,4-Dihydro-3-fluoro-2*H*-1,5-benzodioxepin, D-70209
3-Fluoro-2-methylphenol; Ac, *in* F-60056

$C_9H_9FO_4$
3-Fluoro-2,6-dimethoxybenzoic acid, *in* F-60023
5-Fluoro-2,3-dimethoxybenzoic acid, *in* F-60025

$C_9H_9F_3O_3S$
3-(Trifluoromethyl)benzenesulfonic acid; Et ester, *in* T-60283

$C_9H_9IO_4$
2-Iodo-4,5-dimethoxybenzoic acid, *in* D-60338
3-Iodo-2,4-dimethoxybenzoic acid, *in* D-60331
3-Iodo-2,6-dimethoxybenzoic acid, *in* D-60334
3-Iodo-4,5-dimethoxybenzoic acid, *in* D-60335
4-Iodo-2,5-dimethoxybenzoic acid, *in* D-60333
5-Iodo-2,4-dimethoxybenzoic acid, *in* D-60332
6-Iodo-2,3-dimethoxybenzoic acid, *in* D-60330

$C_9H_9I_3$
1,3,5-Tris(iodomethyl)benzene, T-80366

C_9H_9N
3*a*,7*a*-Methano-1*H*-indole, M-70041
6-Methyl-1*H*-indole, M-60088
3-Phenyl-2-propyn-1-amine, P-60129
5*H*-Pyrrolo[1,2-*a*]azepine, P-70189

C_9H_9NO
3-Amino-1-indanone, A-60211
Bicyclo[4.2.1]nona-2,4,7-trien-9-one; Oxime, *in* B-80084
7,8-Dihydro-5(6*H*)-isoquinolinone, D-60254
1*H*-Indole-6-methanol, I-60032
6-Methoxyindole, *in* H-60158
3-Methoxy-1*H*-isoindole, *in* P-70100
Phthalimidine; *N*-Me, *in* P-70100

C_9H_9NOS
2*H*-1,4-Benzothiazin-3(4*H*)-one; N-Me, *in* B-80043

$C_9H_9NO_2$
5,6-Dihydroxyindole; *N*-Me, *in* D-70307
5-Methoxy-1*H*-indol-6-ol, *in* D-70307
6-Methoxy-1*H*-indol-5-ol, *in* D-70307
1-Nitro-1-phenylpropene, N-80057
4-Phenyl-2-oxazolidinone, P-60126

$C_9H_9NO_3$
1,4-Benzodioxan-6-carboxaldehyde; Oxime, *in* B-60023
1,4-Benzodioxan-2-carboxylic acid; Amide, *in* B-60024
(2-Oxo-2-phenylethyl)carbamic acid, O-70099

$C_9H_9NO_3S$
3-Carboxy-2,3-dihydro-8-hydroxy-5-methylthiazolo[3,2-*a*]pyridinium hydroxide inner salt, C-70021

$C_9H_9NO_4$
2,6-Bis(hydroxyacetyl)pyridine, B-70144
3-Hydroxy-4,5-methylenedioxybenzoic acid; Me ether, amide, *in* H-60178

$C_9H_9NO_5$
3-Amino-4-methoxy-1,2-benzenedicarboxylic acid, *in* A-70151
2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-10388

$C_9H_9NO_6$
4,5-Dihydroxy-2-nitrobenzoic acid; 4-Me ether, Me ester, *in* D-60360
4,5-Dimethoxy-2-nitrobenzoic acid, *in* D-60360

$C_9H_9N_3$
1-Aminophthalazine; *N*-Me, *in* A-70184
4,5-Diaminoisoquinoline, D-70040
5,8-Diaminoisoquinoline, D-70041
4,5-Diaminoquinoline, D-70044
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid; Dinitrile, *in* D-80193
(2-Pyridyl)(1-pyrazolyl)methane, P-70178

$C_9H_9N_3O_2$
1,3(2*H*,4*H*)-Isoquinolinedione; Dioxime, *in* I-70099

$C_9H_9N_3O_3$
Biuret; *N*-Benzoyl, *in* B-60190

$C_9H_9N_3S$
1,2,3-Benzotriazine-4(3*H*)-thione; 2-*N*-Et, *in* B-60050

$C_9H_9N_5$
4-Benzoyl-1,2,3-triazole; Hydrazone, *in* B-70079
▷ 2,4-Diamino-6-phenyl-1,3,5-triazine, D-60041

$C_9H_9N_5O_4$
6-(1,2-Dicarboxyethylamino)purine, D-80115

C_9H_{10}
5,6-Dihydro-4*H*-indene, D-70217
7-Methylene-1,3,5-cyclooctatriene, M-60074
Tricyclo[3.3.1.0^{2,8}]nona-3,6-diene, T-70230

$C_9H_{10}BrNO$
2-Bromo-3-methylaniline; *N*-Ac, *in* B-70234

$C_9H_{10}ClN$
4-Chloro-2,3-dihydro-1*H*-indole; 1-Me, *in* C-60055

$C_9H_{10}ClNO$
2′-Amino-2-chloro-3′-methylacetophenone, A-60112
2′-Amino-2-chloro-4′-methylacetophenone, A-60113
2′-Amino-2-chloro-5′-methylacetophenone, A-60114
2′-Amino-2-chloro-6′-methylacetophenone, A-60115
2-Chloro-4,6-dimethylbenzaldehyde; Oxime, *in* C-60061

$C_9H_{10}FNO_2S$
N-Fluoro-2,3-dihydro-3,3-dimethyl-1,2-benzothiadiazole 1,1-dioxide, F-80032

$C_9H_{10}N_2$
2,3-Dihydro-1*H*-1,4-benzodiazepine, D-80173
4,5-Dihydro-1*H*-pyrazole; 1-Ph, *in* D-70253

$C_9H_{10}N_2O$
3,4-Dihydro-2(1*H*)-quinazolinone; 3-Me, *in* D-60278
▷ 1-Phenyl-3-pyrazolidinone, P-70091
1,3,4,5-Tetrahydro-2*H*-1,3-benzodiazepin-2-one, T-60058

$C_9H_{10}N_2O_2$
2-Acetyl-5-aminopyridine; *N*-Ac, *in* A-70023
1-Carbethoxy-2-cyano-1,2-dihydropyridine, C-70017

$C_9H_{10}N_2O_3$
1,4-Benzodioxan-6-carboxylic acid; Hydrazide, *in* B-60025
2,4-Diaminobenzoic acid; 2-*N*-Ac, *in* D-60032
2,4-Diaminobenzoic acid; 4-*N*-Ac, *in* D-60032

$C_9H_{10}N_2O_4$
5-Amino-3,4-pyridinedicarboxylic acid; Di-Me ester, *in* A-70195
2-Amino-3,5-pyridinedicarboxylic acid; 3-Mono-Et ester, *in* A-70193
2-Amino-3,5-pyridinedicarboxylic acid; 5-Mono-Et ester, *in* A-70193

$C_9H_{10}N_2S$
2-Amino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylic acid; Nitrile, *in* A-60258

$C_9H_{10}N_4$
4-Dimethylamino-1,2,3-benzotriazine, *in* A-60092
2,6,7-Trimethylpteridine, T-70286
4,6,7-Trimethylpteridine, T-70287

$C_9H_{10}N_4O$
4-Amino-1,2,3-benzotriazine; *N*,*N*(4)-Di-Me, 2-Oxide, *in* A-60092
Di-1*H*-imidazol-2-ylmethanone; 1,1′-Di-Me, *in* D-70354

$C_9H_{10}N_4O_3$
2,4,6(1*H*,3*H*,5*H*)-Pteridinetrione; 1,3,5-Tri-Me, *in* P-70134
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1,3,6-Tri-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1,3,8-Tri-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1,6,8-Tri-Me, *in* P-70135
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 3,6,8-Tri-Me, *in* P-70135

$C_9H_{10}N_4O_4$
4-Amino-4,6-dihydro-3-methyl-1*H*-cyclopenta[*e*]1,2,4-triazine-5,7-dicarboxylic acid, A-80066

$C_9H_{10}N_4S$
Tetrazole-5-thione; 3-Et, 1-Ph, *in* T-60174

$C_9H_{10}O$
2,7-Dimethyl-2,4,6-cycloheptatrien-1-one, D-70391
1-Ethenyl-4-methoxybenzene, *in* H-70209
1-Methoxy-1-phenylethylene, *in* P-60092
4-Nonene-6,8-diyn-1-ol, N-80072
1-Phenylcyclopropanol, P-70066
4-(1-Propenyl)phenol, P-80179
3,5,6,7-Tetrahydro-4*H*-inden-4-one, T-70070

$C_9H_{10}OS$
Benzyl vinyl sulfoxide, *in* B-80062
1-[4-(Methylthio)phenyl]ethanone, *in* M-60017
[(Phenylthio)methyl]oxirane, *in* M-80173

$C_9H_{10}OSe$
[2-(Methylseleninyl)ethenyl]benzene, *in* M-70132

$C_9H_{10}O_2$
2-Benzyloxyacetaldehyde, B-70085
Bicyclo[2.2.1]hepta-2,5-diene-2-carboxylic acid; Me ester, *in* B-60084
3,4-Dihydro-2*H*-1-benzopyran-2-ol, D-60198
3,4-Dihydro-2*H*-1-benzopyran-3-ol, D-60199
3,4-Dihydro-2*H*-1-benzopyran-4-ol, D-60200
3,4-Dihydro-2*H*-1-benzopyran-5-ol, D-60201
3,4-Dihydro-2*H*-1-benzopyran-6-ol, D-70175
3,4-Dihydro-2*H*-1-benzopyran-7-ol, D-60202
3,4-Dihydro-2*H*-1-benzopyran-8-ol, D-60203
5-Ethyl-2-hydroxy-2,4,6-cycloheptatrien-1-one, E-70044
2′-(Hydroxymethyl)acetophenone, H-70158
4′-(Hydroxymethyl)acetophenone, H-70159
2-Hydroxy-2-phenylpropanal, H-80240
1-(4-Hydroxyphenyl)-2-propanone, H-80241
2-Methoxybenzeneacetaldehyde, *in* H-60207
α-Methoxybenzeneacetaldehyde, *in* H-60210
2-Methoxy-4-methylbenzaldehyde, *in* H-70160
3-Methoxy-5-methylbenzaldehyde, *in* H-80195
4-Methoxy-2-methylbenzaldehyde, *in* H-70161
4-Methoxyphenylacetaldehyde, *in* H-60209
Spiro[4.4]non-2-ene-1,4-dione, S-60042

$C_9H_{10}O_2S$
Benzyl vinyl sulfone, *in* B-80062
Isopropenyl phenyl sulfone, *in* P-80137
2-Mercapto-2-phenylacetic acid; Me ester, *in* M-60024
2-Mercapto-3-phenylpropanoic acid, M-60026
[2-(Methylsulfonyl)ethenyl]benzene, *in* M-80170
3-(3-Thienyl)-2-propenoic acid; Et ester, *in* T-70172

$C_9H_{10}O_2Se$
[2-(Methylselenonyl)ethenyl]benzene, *in* M-70132

$C_9H_{10}O_3$
Bicyclo[3.3.1]nonane-2,4,7-trione, B-80082
Bicyclo[3.3.1]nonane-2,4,9-trione, B-80083
2-Ethoxybenzoic acid, *in* H-70108
▷ Ethyl salicylate, *in* H-70108
4-Hydroxybenzyl alcohol; α-Ac, *in* H-80114
3-Hydroxy-4-methoxyphenylacetaldehyde, *in* D-60371
4-Hydroxy-3-methoxyphenylacetaldehyde, *in* D-60371
2-(Hydroxymethyl)-1,4-benzodioxan, H-60172
2-Hydroxy-4-methylbenzoic acid; Me ester, *in* H-70163
2-Methoxy-4-methylbenzoic acid, *in* H-70163
4-Methoxy-2-methylbenzoic acid, *in* H-70164

$C_9H_{10}O_4$
2,6-Dihydroxy-3,5-dimethylbenzoic acid, D-70293
2′,6′-Dihydroxy-4′-methoxyacetophenone, *in* T-70248
2-(3,4-Dihydroxyphenyl)propanoic acid, D-60372
2,3-Dimethoxy-5-methyl-1,4-benzoquinone, *in* D-70320
Glycol salicylate, *in* H-70108
(2-Hydroxyphenoxy)acetic acid; Me ester, *in* H-70203
Methoxymethyl salicylate, *in* H-70108
(2-Methoxyphenoxy)acetic acid, *in* H-70203
(3-Methoxyphenoxy)acetic acid, *in* H-70204
(4-Methoxyphenoxy)acetic acid, *in* H-70205
2′,4′,6′-Trihydroxy-3′-methylacetophenone, T-80321
3-(3,4,5-Trihydroxyphenyl)propanal, T-80333

$C_9H_{10}O_4S$
2*H*-Thiopyran-2,2-dicarboxylic acid; Di-Me ester, *in* T-80191

$C_9H_{10}O_5$
3,4-Dihydroxy-5-methoxybenzeneacetic acid, *in* T-60343
3,5-Dihydroxy-4-methoxybenzeneacetic acid, *in* T-60343
5-Hydroxy-2,3-dimethoxybenzoic acid, *in* T-70250
3,4,6-Trihydroxy-2-methylbenzoic acid; Me ester, *in* T-80324
3,4,5-Trihydroxyphenylacetic acid; Me ester, *in* T-60343

$C_9H_{10}O_6$
3,5-Dihydroxy-4-oxo-4*H*-pyran-2-carboxylic acid; Di-Me ether, Me ester, *in* D-60368

$C_9H_{10}S$
Benzyl vinyl sulfide, B-80062
[1-(Methylthio)ethenyl]benzene, M-80169
[2-(Methylthio)ethenyl]benzene, M-80170

$C_9H_{10}S_2$
1,5-Dihydro-2,4-benzodithiepin, D-60194
3,4-Dihydro-2*H*-1,5-benzodithiepin, D-60195

$C_9H_{10}Se$
[2-(Methylseleno)ethenyl]benzene, M-70132

$C_9H_{11}BrO_3$
1-Bromo-2,3,4-trimethoxybenzene, *in* B-60200
1-Bromo-2,3,5-trimethoxybenzene, *in* B-70182
1-Bromo-2,4,5-trimethoxybenzene, *in* B-70181
2-Bromo-1,3,4-trimethoxybenzene, *in* B-70180
2-Bromo-1,3,5-trimethoxybenzene, *in* B-60199
5-Bromo-1,2,3-trimethoxybenzene, *in* B-60201

$C_9H_{11}N$
Azetidine; *N*-Ph, *in* A-70283
Bicyclo[2.2.2]oct-2-ene-1-carboxylic acid; Nitrile, *in* B-70113
1,2,3,4-Tetrahydroquinoline, T-70093

$C_9H_{11}NO$
2-(Dimethylamino)benzaldehyde, D-60401
N-Methylbenzenecarboximidic acid; Me ester, *in* M-60045
1,2,3,4-Tetrahydro-4-hydroxyisoquinoline, T-60066
1,2,3,4-Tetrahydro-5-hydroxyisoquinoline, T-80065
1,2,3,4-Tetrahydro-7-hydroxyisoquinoline, T-80066
6,7,8,9-Tetrahydro-4*H*-quinolizin-4-one, T-60092

$C_9H_{11}NOS$
2-(1,3-Oxathian-2-yl)pyridine, O-60049

$C_9H_{11}NO_2$
▷ 2-Ethoxybenzamide, *in* H-70108
2-Hydroxyphenylacetaldehyde; Me ether, oxime, *in* H-60207
3-Hydroxyphenylacetaldehyde; Me ether, oxime, *in* H-60208
4-Hydroxyphenylacetaldehyde; Me ether, oxime, *in* H-60209
N-Methylphenylacetohydroxamic acid, *in* P-70059
3*a*,4,7,7*a*-Tetrahydro-1*H*-isoindole-1,3(2*H*)-dione; *N*-Me, *in* T-80070

$C_9H_{11}NO_2S$
2-Amino-3-mercapto-3-phenylpropanoic acid, A-60213
2-Amino-3-(4-mercaptophenyl)propanoic acid, A-60214
2-Amino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylic acid, A-60258

$C_9H_{11}NO_3$
4-Amino-1,2-benzenediol; O^1-Me, 2-Ac, *in* A-70090
4-Amino-1,2-benzenediol; O^2-Me, 1-Ac, *in* A-70090
3-Amino-3-(4-hydroxyphenyl)propanoic acid, A-80084
2,3-Dihydroxybenzaldehyde; Di-Me ether, oxime, *in* D-70285
2,4-Dihydroxyphenylacetaldehyde; Di-Me ether, oxime, *in* D-60369
3,4-Dihydroxyphenylacetaldehyde; 3-Me ether, oxime, *in* D-60371
(2-Hydroxyphenoxy)acetic acid; Me ether, amide, *in* H-70203

$C_9H_{11}NO_4$
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid, D-80193

$C_9H_{11}NO_5$
3-Hydroxy-1*H*-pyrrole-2,5-dicarboxylic acid; Me ether, Di-Me ester, *in* H-80252
1*H*-Pyrrole-3,4-dicarboxylic acid; 1-Methoxy, Di-Me ester, *in* P-70183

$C_9H_{11}NS$
2-(Tetrahydro-2-thienyl)pyridine, T-60097
2,3,4,5-Tetrahydrothiepino[2,3-*b*]pyridine, T-60098

$C_9H_{11}NS_2$
2-(1,3-Dithian-2-yl)pyridine, D-60504

$C_9H_{11}N_5$
5-Amino-1*H*-tetrazole; 1-Me, 4-Benzyl, *in* A-70202
5-Amino-1*H*-tetrazole; 2-Me, 5-*N*-Benzyl, *in* A-70202
1-Benzyl-5-imino-3-methyl-1*H*,3*H*-tetrazole, *in* A-70202
3-Benzyl-5-imino-1-methyl-1*H*,3*H*-tetrazole, *in* A-70202
1-Benzyl-5-methylamino-1*H*-tetrazole, *in* A-70202

$C_9H_{11}N_5O_2$
6-Acetylhomopterin, A-70043
Deoxysepiapterin, *in* S-70035

$C_9H_{11}N_5O_3$
Biopterin, B-70121
Sepiapterin, S-70035

C_9H_{12}
Bicyclo[3.3.1]nona-2,6-diene, B-70102
2,3-Dimethylenebicyclo[2.2.1]heptane, D-70405
▷ 5-Ethenylbicyclo[2.2.1]hept-2-ene, E-70036
1-Ethynylcycloheptene, E-70050
1,3-Nonadiyne, N-80069
1,3,5,7-Nonatetraene, N-70071
Trispiro[2.0.2.0.2.0]nonane, T-70325

$C_9H_{12}ClN_3O_4$
5′-Chloro-5′-deoxyarabinosylcytosine, C-70064

$C_9H_{12}N_2$
6,7,8,9-Tetrahydro-5*H*-pyrido[2,3-*b*]azepine, T-70091
6,7,8,9-Tetrahydro-5*H*-pyrido[3,2-*b*]azepine, T-70092

$C_9H_{12}N_2O$
Acetamidoxime; *O*-Benzyl, *in* A-60016

4-Acetyl-2-aminopyridine; N^2,N^2-Di-Me, *in* A-70026
2-(Dimethylamino)benzaldehyde; Oxime, *in* D-60401

$C_9H_{12}N_2OS$
2-Amino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylic acid; Amide, *in* A-60258

$C_9H_{12}N_2O_2$
2,4,6-Trimethyl-3-nitroaniline, T-70285

$C_9H_{12}N_2O_3$
2-Amino-3-nitrobenzyl alcohol; *N*-Et, *in* A-80125
3-Amino-2-nitrobenzyl alcohol; *N*-Et, *in* A-80127
3-Amino-4-nitrobenzyl alcohol; *N*-Et, *in* A-80128

$C_9H_{12}N_4O_5$
5-Nitrohistidine; Me ester, N^{α}-Ac, *in* N-60028

$C_9H_{12}N_6$
2,3,6,7,10,11-Hexahydrotrisimidazo[1,2-*a*;1′,2′-*c*;1″,2″-*e*][1,3,5]-triazine, H-60061

$C_9H_{12}O$
Bicyclo[3.3.1]non-3-en-2-one, B-70105
Bicyclo[4.2.1]non-2-en-9-one, B-70106
Bicyclo[4.2.1]non-3-en-9-one, B-70107
Bicyclo[4.2.1]non-7-en-9-one, B-70108
3*a*,4,5,6,7,7*a*-Hexahydro-1*H*-inden-1-one, H-70058
Isopropyl phenyl ether, I-80085
3,4,5-Trimethylphenol, T-60371

$C_9H_{12}O_2$
Bicyclo[3.3.1]nonane-2,4-dione, B-70103
Bicyclo[2.2.2]oct-2-ene-1-carboxylic acid, B-70113
2-Carbomethoxy-3-vinylcyclopentene, *in* V-60010
1,3-Diacetylbicyclo[1.1.1]pentane, D-80041
2,2-Dimethyl-5-cycloheptene-1,3-dione, D-60416
3-Ethynyl-3-methyl-4-pentenoic acid; Me ester, *in* E-60059
2,3,4,4*a*,5,6-Hexahydro-7*H*-1-benzopyran-7-one, H-60045
3*a*,4,5,6,7,7*a*-Hexahydro-3-methylene-2-(3*H*)-benzofuranone, H-70062
4-Hydroxybenzyl alcohol; Di-Me ether, *in* H-80114
4-Nonen-2-ynoic acid, N-70072
1-Phenyl-1,2-propanediol, P-80121
1-Phenyl-1,3-propanediol, P-80122

$C_9H_{12}O_3$
1,3,5-Cyclohexanetricarboxaldehyde, C-70226
6-Ethyl-4-hydroxy-3,5-dimethyl-2*H*-pyran-2-one, E-80065
Hexahydro-1*H*-2-benzopyran-1,3(4*H*)-dione, *in* C-8[illegible]
1-Hydro[illegible]yclohexene-1-carboxaldehyde; Ac, *in* [illegible] 146
Metacrolein, [illegible] P-70119
4-Oxo-1-cyclcheptene-1-carboxylic acid; Me ester, *in* O-70082

$C_9H_{12}O_4$
Aucubigenin, A-80186
Bicyclo[1.1.1]pentane-1,3-dicarboxylic acid; Di-Me ester, *in* B-80090
4-Cyclopentene-1,3-diol; Di-Ac, *in* C-80193
4-Cyclopentene-1,3-diol; Mono-Ac, *in* C-80193
5,5-Dimethyl-2-hexynedioic acid; Di-Me ester, *in* D-70415
5-Ethyl-3-hydroxy-4-methyl-2(5*H*)-furanone; Ac, *in* E-60051
Jiofuran, J-80009
2,3,6-Trimethoxyphenol, *in* B-60014
Vertipyronol, V-80005
2-Vinyl-1,1-cyclopropanedicarboxylic acid; Di-Me ester, *in* V-60011

$C_9H_{12}O_5$
4-Oxo-2-heptenedioic acid; Di-Me ester, *in* O-60072
Rehmaglutin *C*, R-60003
Vertipyronediol, *in* V-80005

$C_9H_{12}O_6$
Aconitic acid; Tri-Me ester, *in* A-70055

$C_9H_{12}S_2$
2-Methyl-1,3-benzenedimethanethiol, M-70050

$C_9H_{12}S_3$
1,3,5-Benzenetrimethanethiol, B-70019

$C_9H_{13}NO$
1,2,3,6,7,9*a*-Hexahydro-4(1*H*)-quinolizinone, H-70074
3,4,6,7,8,9-Hexahydro-2*H*-quinolizin-2-one, H-60059

$C_9H_{13}NO_2$
2,4-Diethoxypyridine, *in* H-60224
2,5-Diethoxypyridine, *in* H-60225
2,6-Diethoxypyridine, *in* H-60226
3,4-Diethoxypyridine, *in* H-60227
Hexahydro-1,3(2*H*,4*H*)-isoquinolinedione, H-80060

$C_9H_{13}N_3$
1,2,12-Triazapentacyclo[6.4.0.0^{2,17}.0^{3,7}.0^{4,11}]dodecane, T-70205

$C_9H_{13}N_3O_3$
4-Amino-5-methyl-1*H*-pyrazole-3-carboxylic acid; *N*-Ac, Et ester, *in* A-80111
5-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Me, *N*(5)-Ac, Et ester, *in* A-70192
2′,3′-Dideoxycytidine, D-80152

$C_9H_{13}N_5$
2-(Diethylamino)purine, *in* A-60243

$C_9H_{13}N_5O_6$
Clitocine, C-60155

C_9H_{14}
7,7-Dimethylbicyclo[4.1.0]hept-3-ene, D-60409
1-Isopropenylcyclohexene, I-60115
3-Isopropenylcyclohexene, I-60116
4-Isopropenylcyclohexene, I-60117
2,3,5-Nonatriene, N-80071
3-Nonen-1-yne, N-80073
1-(1-Propenyl)cyclohexene, P-60178
1-(2-Propenyl)cyclohexene, P-60179
3-(2-Propenyl)cyclohexene, P-60180
4-(1-Propenyl)cyclohexene, P-60181
4-(2-Propenyl)cyclohexene, P-60182

$C_9H_{14}ClNO$
7-Aminobicyclo[2.2.1]heptane; *N*-Chloroacetyl, *in* A-80061

$C_9H_{14}Cl_2O_2$
2,2-Dichloro-6-heptenoic acid; Et ester, *in* D-80119

$C_9H_{14}N_2O_5$
α-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid, A-70120
3,4-Dihydro-2(1*H*)-pyrimidinone; 1-β-D-Ribofuranosyl, *in* D-60273
3,4-Dihydro-2(1*H*)-pyrimidinone; 3-β-D-Ribofuranosyl, *in* D-60273

$C_9H_{14}N_4$
2,3,5,6,8,9-Hexahydro-1*H*-diimidazo[1,2-*d*:2′,1′-*g*][1,4]diazepine, H-80058

$C_9H_{14}N_4O_3$
Caffeidine; Ac, *in* C-60003
Carnosine, C-60020

$C_9H_{14}N_4O_5$
▷ N^4-Aminocytidine, A-70127

$C_9H_{14}O$
1-Acetylcycloheptene, A-60026
2-(1-Cyclohexenyl)propanal, C-80183
1-Cyclooctenecarboxaldehyde, C-60217
2-Oxatricyclo[3.3.1.1^{3,7}]decane, O-60051
2,2,5,5-Tetramethyl-3-cyclopenten-1-one, T-60140
2,3,4-Trimethyl-2-cyclohexen-1-one, T-60359

$C_9H_{14}OS_3$
Ajoene, A-70079

$C_9H_{14}O_2$
Bicyclo[2.2.1]heptane-1-carboxylic acid; Me ester, *in* B-60085
Bicyclo[2.2.2]octane-1-carboxylic acid, B-60092
Bicyclo[3.2.1]octane-1-carboxylic acid, B-70112
1-Cycloheptenecarboxylic acid; Me ester, *in* C-80178
7-Ethyl-5-methyl-6,8-dioxabicyclo[3.2.1]oct-3-ene, E-60052
1-Methyl-2-cyclohexen-1-ol; Ac, *in* M-80065
7-Methylene-1,4-dioxaspiro[4.5]decane, *in* M-80081
5-Methyl-2,4-hexadienoic acid; Et ester, *in* M-70086
Mitsugashiwalactone, M-70150
2,6-Octadienoic acid; Me ester, *in* O-80011
Octahydro-1*H*-2-benzopyran-1-one, O-80012
Octahydro-7*H*-1-benzopyran-7-one, O-60011
4-Oxo-2-nonenal, O-70097

$C_9H_{14}O_2S$
2-Thiatricyclo[3.3.1.1^{3,7}]decane; 2,2-Dioxide, *in* T-60195

$C_9H_{14}O_3$
2-*tert*-Butyl-2,4-dihydro-6-methyl-1,3-dioxol-4-one, B-60345
2-*tert*-Butylpentanedioic acid; Anhydride, *in* B-80289
2,3-Diisopropoxycyclopropenone, *in* D-70290
2-(3,3-Dimethoxypropyl)furan, *in* F-80089
3-Oxocyclopentaneacetic acid; Et ester, *in* O-70083

$C_9H_{14}O_4$
2-Carboxycyclohexaneacetic acid, C-80023
1,2-Cyclopentanediol; Di-Ac, *in* C-80189
1,1-Cyclopropanedicarboxylic acid; Di-Et ester, *in* C-80196
2-Hydroxycyclohexanecarboxylic acid; Ac, *in* H-70119
Jioglutolide, J-80012

$C_9H_{14}O_5$
Bissetone, B-60174
4-Oxoheptanedioic acid; Di-Me ester, *in* O-60071
4,4-Pyrandiacetic acid, P-70150

$C_9H_{14}S$
2,2,5,5-Tetramethyl-3-cyclopentene-1-thione, T-60139
2-Thiatricyclo[3.3.1.1^{3,7}]decane, T-60195

$C_9H_{15}ClO_2$
7-Chloro-2-heptenoic acid; Et ester, *in* C-70069

$C_9H_{15}N$
▷ Tri(2-propenyl)amine, T-70315

$C_9H_{15}NO$
7-Aminobicyclo[2.2.1]heptane; *N*-Ac, *in* A-80061
3-Aminobicyclo[2.2.1]hept-5-ene-2-methanol; *N*-Me, *in* A-70094
3,6-Dihydro-3,3,6,6-tetramethyl-2(1*H*)-pyridinone, D-70267
Octahydro-4*H*-quinolizin-4-one, O-60019
2-(2-Propenyl)cyclohexanone; Oxime, *in* P-80177

$C_9H_{15}NO_2$
7-Aminobicyclo[2.2.1]heptane; *N*-Methoxycarbonyl, *in* A-80061
3-*tert*-Butyl-2,6-piperidinedione, *in* B-80289
3,4-Dihydro-2*H*-pyrrole-5-carboxylic acid; *tert*-Butyl ester, *in* D-80249

$C_9H_{15}NO_3$
2-Amino-2-hexenoic acid; *N*-Ac, Me ester, *in* A-60167
Methyl 3-*tert*-butylamino-2-formyl-2-propenoate, *in* A-80134
5-Oxo-2-pyrrolidinecarboxylic acid; *tert*-Butyl ester, *in* O-70102

$C_9H_{15}NO_5$
4-Oxoheptanedioic acid; Di-Me ester, oxime, *in* O-60071

$C_9H_{15}N_3$
3,5,12-Triazatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane, T-70206
2,4,6-Triethyl-1,3,5-triazine, T-70235

$C_9H_{15}N_3O_2$
Histidine trimethylbetaine, H-60083

$C_9H_{15}N_3O_2S$
Ovothiol *C*, *in* O-70050

$C_9H_{15}N_3O_3$
Triethyl isocyanurate, *in* C-60179

$C_9H_{15}N_3O_8$
Hexahydro-1,3,5-triazine; 1,3,5-Tri-Ac, *in* H-60060

$C_9H_{15}N_3O_{11}P_2$
Cytidine-5′-diphosphate, C-80204

C_9H_{16}
1-*tert*-Butylcyclopentene, B-70298
3-*tert*-Butylcyclopentene, B-70299
4-*tert*-Butylcyclopentene, B-70300
1-Isopropylcyclohexene, I-60118
3-Isopropylcyclohexene, I-60119
4-Isopropylcyclohexene, I-60120

$C_9H_{16}Br_2$
2,2-Dibromo-1,1,3,3-tetramethylcyclopentane, D-80102

$C_9H_{16}Br_4$
Tetrakis(2-bromoethyl)methane, T-70124

$C_9H_{16}N_2$
2-Diazo-1,1,3,3-tetramethylcyclopentane, D-60066
2,2,5,5-Tetramethyl-3-cyclopenten-1-one; Hydrazone, *in* T-60140

$C_9H_{16}N_2O_2$
3-(2-Methylpropyl)-6-methyl-2,5-piperazinedione, M-70118
3,5-Pyrazolidinedione; 1,2-Dipropyl, *in* P-80200

$C_9H_{16}N_2O_4S$
S-(2-Aminoethyl)cysteine; N^{α},N^{ϵ}-Di-Ac, *in* A-60152

$C_9H_{16}N_2O_5$
N,*N*′-Carbonylbisglycine; Di-Et ester, *in* C-80020
Tetrahydro-2(1*H*)-pyrimidinone; 1-β-D-Ribofuranosyl, *in* T-60088
Tetrahydro-2(1*H*)-pyrimidinone; 1-β-D-Ribopyranosyl, *in* T-60088

$C_9H_{16}N_3O_{14}P_3$
Cytidine 5′-triphosphate, C-80205

$C_9H_{16}O$
3-*tert*-Butylbicyclo[3.1.0]hexane, B-70294
2-Cyclohexylpropanal, C-80184
2-Methylcyclooctanone, M-60059
2-Methyl-2-octenal, M-60106
6,8-Nonadien-1-ol, N-80068
2-Nonyn-1-ol, N-80074
2,2,5,5-Tetramethylcyclopentanone, T-60138
2,2,5-Trimethyl-4-hexen-3-one, T-60366

$C_9H_{16}OS$
Octahydro-2*H*-1-benzothiopyran; 1α-Oxide, *in* O-80013
Octahydro-2*H*-1-benzothiopyran; 1β-Oxide, *in* O-80013

$C_9H_{16}O_2$
▷ Dihydro-5-pentyl-2(3*H*)-furanone, D-70245
2,7-Dimethoxycycloheptene, *in* C-80179
5,5-Dimethoxy-3,3-dimethyl-1-pentyne, *in* D-80467
1,1-Dimethoxy-3-methylenecyclohexane, *in* M-80081
1,3-Dimethyl-2,9-dioxabicyclo[3.3.1]nonane, D-80445
4,4-Dimethyl-6-heptenoic acid, D-80450
3,3-Dimethyl-4-pentenoic acid; Et ester, *in* D-60437
3,9-Dioxaspiro[5.5]undecane, D-70462
2-Ethyl-1,6-dioxaspiro[4.4]nonane, E-70043
2-Hydroxycyclononanone, H-60112
3-Hydroxycyclononanone, H-60113
2-Methyl-1,6-dioxaspiro[4.5]decane, M-60062
7-Methyl-1,6-dioxaspiro[4.5]decane, M-80069
2-Methyl-4-hexenoic acid; Et ester, *in* M-80100
2-Methyl-5-hexen-1-ol; Ac, *in* M-80104
(Tetrahydro-4-methyl-2*H*-pyran-2-yl)-2-propanone, T-80074
1,2,5-Trimethylcyclopentanecarboxylic acid, T-60361
2,2,5-Trimethylcyclopentanecarboxylic acid, T-60360

$C_9H_{16}O_2S$
Octahydro-2*H*-1-benzothiopyran; 1,1-Dioxide, *in* O-80013

$C_9H_{16}O_3$
2-Cyclohexyl-2-hydroxyacetic acid; Me ester, *in* C-60212
2-Cyclohexyl-2-methoxyacetic acid, *in* C-60212
3,3-Dimethyl-4-oxopentanoic acid; Et ester, *in* D-60433
2-Hydroxycyclooctanecarboxylic acid, H-70121
9-Hydroxy-5-nonenoic acid, H-70194

$C_9H_{16}O_4$
2-*tert*-Butylpentanedioic acid, B-80289
(1-Methylpropyl)propanedioic acid; Di-Me ester, *in* M-70119
2,3-Pentanediol; Di-Ac, *in* P-80060

$C_9H_{16}O_7$
1,5-Dioxiranyl-1,2,3,4,5-pentanepentol, D-70465

$C_9H_{16}S$
Octahydro-2*H*-1-benzothiopyran, O-80013

$C_9H_{16}Se$
2,2,5,5-Tetramethylcyclopentaneselone, T-60137

$C_9H_{17}Br$
1-Bromo-3-nonene, B-60310

$C_9H_{17}NO$
3-Aminobicyclo[2.2.1]heptane-2-methanol; *N*-Me, *in* A-70093
Hexahydro-5(2*H*)-azocinone; 1-Et, *in* H-70048
Octahydro-2*H*-1,3-benzoxazine; *N*-Me, *in* O-70011
Octahydro-1-methyl-2*H*-3,1-benzoxazine, *in* O-70012
Tetrahydro-2-(2-piperidinyl)furan, T-60082
2,2,5-Trimethylcyclopentanecarboxylic acid; Amide, *in* T-60360

$C_9H_{17}NO_2$
2-Acetylpiperidine; Ethylene ketal, *in* A-70051
1,4-Dioxa-8-azaspiro[4.7]dodecane, *in* H-70047
1,4-Dioxa-9-azaspiro[4.7]dodecane, *in* H-70048
2-Methyl-2-piperidinecarboxylic acid; Et ester, *in* M-60119
Stachydrine ethyl ester, *in* S-60050

$C_9H_{17}NO_2S$
2-Thiazolidineacetic acid; *tert*-Butyl ester, *in* T-80173

$C_9H_{17}NO_3$
2-Amino-4,4-dimethylpentanoic acid; *N*-Ac, *in* A-70137
2-Amino-3-hydroxy-4-methyl-6-octenoic acid, A-60189
8-Amino-7-oxononanoic acid, A-80130

$C_9H_{17}NO_4$
2-Amino-3-methylbutanedioic acid; Di-Et ester, *in* A-70166
3-(Carboxymethylamino)propanoic acid; Di-Et ester, *in* C-60016
▷ Levocarnitine; *O*-Ac, *in* C-70024

$C_9H_{17}NO_8$
▷ Miserotoxin, *in* N-60039

$C_9H_{18}Br_2$
3,3-Dibromo-2,2,4,4-tetramethylpentane, D-80104

$C_9H_{18}ClNO$
2,2,6,6-Tetramethyl-1-oxopiperidinium (1+); Chloride, *in* T-80147

$C_9H_{18}Cl_2$
3,3-Dichloro-2,2,4,4-tetramethylpentane, D-80137

$C_9H_{18}NO^{\oplus}$
2,2,6,6-Tetramethyl-1-oxopiperidinium (1+), T-80147

$C_9H_{18}N_2$
1,5-Diazabicyclo[5.2.2]undecane, D-60055
N-(2,2,6,6-Tetramethylpiperidyl)nitrene, T-80149

$C_9H_{18}N_2O_2$
▷ 3-[(3-Methylbutyl)nitrosoamino]-2-butanone, M-60055
2,4-Pentanediamine; N^2,N^4-Di-Ac, *in* P-70039

$C_9H_{18}N_2O_4S$
N-Serylmethionine; Me ester, *in* S-60024

$C_9H_{18}N_6$
1,3,5-Cyclohexanetricarboxaldehyde; Trishydrazone, *in* C-70226

$C_9H_{18}O$
1-Nonen-3-ol, N-60058

$C_9H_{18}O_2$
4,4-Diethoxy-2-methyl-2-butene, *in* M-70055
4,4-Dimethylpentanoic acid; Et ester, *in* D-70428

$C_9H_{18}O_3$
6-Hydroxy-2,4-dimethylheptanoic acid, H-60121
2,4,6-Triethyl-1,3,5-trioxane, T-80266
1,5,9-Trioxacyclododecane, T-70304

$C_9H_{18}O_4$
Ethyl 3,3-diethoxypropionate, *in* O-60090

$C_9H_{19}N$
Octahydroazocine; 1-Et, *in* O-70010

$C_9H_{19}NO$
2-Amino-4-*tert*-butylcyclopentanol, A-70104
2-(Aminomethyl)cyclooctanol, A-70170

$C_9H_{19}NS_2$
2-Pyrrolidinecarboxaldehyde; Diethyl dithioacetal, *in* P-70184

$C_9H_{20}ClNO_2$
▷ Muscarine; Chloride, *in* M-60153

$C_9H_{20}INO_2$
Muscarine; Iodide, *in* M-60153

$C_9H_{20}NO_2^{\oplus}$
▷ Muscarine, M-60153

$C_9H_{20}NO_3^{\oplus}$
4-Ethoxy-2-hydroxy-*N*,*N*,*N*-trimethyl-4-oxo-1-butanaminium, *in* C-70024

$C_9H_{20}N_2$
4-Amino-2,2,6,6-tetramethylpiperidine, A-70201

$C_9H_{20}N_2O_3$
N,*N*′-[Carbonylbis(oxy)]bis[2-methyl-2-propanamine], *in* C-60015

$C_9H_{20}O$
2,2,4,4-Tetramethyl-3-pentanol, T-80148

$C_9H_{20}O_4S_4$
Tetrakis(methylsulfinylmethyl)methane, *in* B-60164

$C_9H_{20}S_4$
Tetrakis(methylthiomethyl)methane, *in* B-60164

$C_9H_{21}N_3$
▷ Hexahydro-1,3,5-triazine; 1,3,5-Tri-Et, *in* H-60060
1,4,7-Triazacyclododecane, T-60231
1,5,9-Triazacyclododecane, T-60232

$C_{10}Cl_{12}$
▷ Dodecachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{5,8}]decane, D-70530

$C_{10}F_8$
Octafluoronaphthalene, O-70008

$C_{10}F_{11}IO_4$
[Bis(trifluoroacetoxy)iodo]pentafluorobenzene, B-80161

$C_{10}HF_7$
1,2,3,4,5,6,7-Heptafluoronaphthalene, H-70019
1,2,3,4,5,6,8-Heptafluoronaphthalene, H-70020

$C_{10}H_2F_4$
1,3-Diethynyl-2,4,5,6-tetrafluorobenzene, D-70159
1,4-Diethynyl-2,3,5,6-tetrafluorobenzene, D-70160

$C_{10}H_2F_6$
1,2,3,4,5,6-Hexafluoronaphthalene, H-70044
1,2,4,5,6,8-Hexafluoronaphthalene, H-70045

$C_{10}H_4^{2\ominus}$
Dihydrocyclopenta[*c,d*]pentalene(2−), D-60216

$C_{10}H_4Br_2O_2$
6,7-Dibromo-1,4-naphthoquinone, D-70096

$C_{10}H_4Cl_2FNO_2$
3,4-Dichloro-1-(4-fluorophenyl)-1*H*-pyrrole-2,5-dione, D-60132

$C_{10}H_4Cl_2O_2$
6,7-Dichloro-1,4-naphthoquinone, D-70124

$C_{10}H_4F_6$
1,4-Bis(trifluorovinyl)benzene, B-80165

$C_{10}H_4K_2$
Dihydrocyclopenta[*c,d*]pentalene(2−); Di-K salt, *in* D-60216

$C_{10}H_4O_2S_2$
Benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-dione, B-60031

$C_{10}H_4S_8$
Bi(1,3-dithiolo[4,5-*b*][1,4]dithiin-2-ylidene), B-70118

$C_{10}H_5BrO_3$
2-Bromo-3-hydroxy-1,4-naphthoquinone, B-60268
2-Bromo-5-hydroxy-1,4-naphthoquinone, B-60269
2-Bromo-6-hydroxy-1,4-naphthoquinone, B-60270
2-Bromo-7-hydroxy-1,4-naphthoquinone, B-60271
2-Bromo-8-hydroxy-1,4-naphthoquinone, B-60272
7-Bromo-2-hydroxy-1,4-naphthoquinone, B-60273
8-Bromo-2-hydroxy-1,4-naphthoquinone, B-60274

$C_{10}H_5Br_2NO_2$
6,7-Dibromo-1-nitronaphthalene, D-70098

$C_{10}H_5ClO_3$
2-Chloro-6-hydroxy-1,4-naphthoquinone, C-80066
2-Chloro-7-hydroxy-1,4-naphthoquinone, C-80067

$C_{10}H_5F_3O$
1,1,1-Trifluoro-4-phenyl-3-butyn-2-one, T-70244

$C_{10}H_5NO_4$
6-Nitro-1,4-naphthoquinone, N-60035
7-Nitro-1,2-naphthoquinone, N-60036

$C_{10}H_5NO_5$
2-Hydroxy-3-nitro-1,4-naphthoquinone, H-60195

$C_{10}H_5N_3O_2$
1*H*-Naphtho[2,3-*d*]triazole-4,9-dione, N-60011

$C_{10}H_6$
1,3-Diethynylbenzene, D-70156
1-Phenyl-1,3-butadiyne, P-80095

$C_{10}H_6Br_2O$
6,7-Dibromo-1-naphthol, D-70095

$C_{10}H_6ClNO_2$
▷ 2-Amino-3-chloro-1,4-naphthoquinone, A-70122

$C_{10}H_6F_3NO_2$
7-Amino-4-(trifluoromethyl)-2*H*-1-benzopyran-2-one, A-60265

$C_{10}H_6F_4O_4$
2,3,5,6-Tetrafluoro-1,4-benzenedicarboxylic acid; Di-Me ester, *in* T-70029

$C_{10}H_6N_2O$
Benzofuro[2,3-*b*]pyrazine, B-80023
2-Cyano-3-hydroxyquinoline, *in* H-60228

$C_{10}H_6N_2OS$
[1,4]Oxathiino[3,2-*b*:5,6-*c'*]dipyridine, O-60050

$C_{10}H_6N_2OSe$
[1,4]Oxaselenino[2,3-*b*:5,6-*b'*]dipyridine, O-70065
[1,4]Oxaselenino[3,2-*b*:5,6-*b'*]dipyridine, O-70066
[1,4]Oxaselenino[3,2-*b*:5,6-*c'*]dipyridine, O-70067
[1,4]Oxaselenino[3,2-*b*:6,5-*c'*]dipyridine, O-70068

$C_{10}H_6N_2O_2$
[1]Benzopyrano[3,4-*c*]pyrazol-4(3*H*)-one, B-80036
3,4-Cinnolinedicarboxaldehyde, C-70180
3,8-Dihydrocyclobuta[*b*]quinoxaline-1,2-dione, D-70178
▷ 1,4-Diisocyanatocubane, D-80406

$C_{10}H_6N_2O_2S$
[1,4]Oxathiino[3,2-*b*:5,6-*c'*]dipyridine; 8-Oxide, *in* O-60050

$C_{10}H_6N_2O_2Se$
[1,4]Oxaselenino[3,2-*b*:5,6-*c'*]dipyridine; 8-Oxide, *in* O-70067
[1,4]Oxaselenino[3,2-*b*:6,5-*c'*]dipyridine; 7-Oxide, *in* O-70068

$C_{10}H_6N_2O_4$
7-Nitro-4-nitroso-1-naphthol, *in* N-60035

$C_{10}H_6N_2S$
Thieno[2,3-*c*]cinnoline, T-60202
Thieno[3,2-*c*]cinnoline, T-60203

$C_{10}H_6N_2S_2$
[1,4]Dithiino[2,3-*b*:6,5-*b'*]dipyridine, D-70519
1,4-Dithiino[2,3-*b*:5,6-*c'*]dipyridine, D-70518
1,4-Dithiino[2,3-*b*:6,5-*c'*]dipyridine, D-70520
Thiazolo[4,5-*b*]quinoline-2(3*H*)-thione, T-60201

$C_{10}H_6N_4O_2$
Pyrazino[2,3-*f*]quinazoline-8,10-(7*H*,9*H*)-dione, P-60201
Pyrazino[2,3-*g*]quinazoline-2,4-(1*H*,3*H*)-dione, P-60200

$C_{10}H_6N_6$
Pyridazino[1″,6″:1′,2′]imidazo[4′,5′:4,5]imidazo[1,2-*b*]pyridazine, P-70169

$C_{10}H_6O_3$
2,3-Epoxy-2,3-dihydro-1,4-naphthoquinone, E-70011
4-Hydroxy-1,2-naphthoquinone, H-60194

$C_{10}H_6O_3Se_2$
Naphth[1,8-*cd*][1,2,6]oxadiselenin 1,3-dioxide, *in* N-80002

$C_{10}H_6O_4$
2,5-Dihydroxy-1,4-naphthoquinone, D-60354
2,8-Dihydroxy-1,4-naphthoquinone, D-60355
▷ 5,8-Dihydroxy-1,4-naphthoquinone, D-60356
6,7-Methylenedioxy-2*H*-1-benzopyran-2-one, M-70068

$C_{10}H_6O_7$
2,3,5,6,8-Pentahydroxy-1,4-naphthoquinone, P-70033

$C_{10}H_6O_8$
Hexahydroxy-1,4-naphthoquinone, H-60065

$C_{10}H_6S_2$
Benzo[1,2-*b*:4,5-*b'*]dithiophene, B-60030

$C_{10}H_6Se_2$
Naphtho[1,8-*cd*]-1,2-diselenole, N-80005

$C_{10}H_6Te_2$
Naphtho[1,8-*cd*]1,2-ditellurole, N-80006

$C_{10}H_7BrN_2$
2-Bromo-3,3′-bipyridine, B-70185
4-Bromo-2,2′-bipyridine, B-70186
5-Bromo-2,3′-bipyridine, B-70187
5-Bromo-2,4′-bipyridine, B-70188
5-Bromo-3,3′-bipyridine, B-70189
5-Bromo-3,4′-bipyridine, B-70190
6-Bromo-2,2′-bipyridine, B-70191
6-Bromo-2,3′-bipyridine, B-70192
6-Bromo-2,4′-bipyridine, B-70193

$C_{10}H_7Br_2N$
6,7-Dibromo-1-naphthylamine, D-70097

$C_{10}H_7Br_3$
1,4,7-Tribromotriquinacene, T-60248

$C_{10}H_7ClN_2$
2-Chloro-3-phenylpyrazine, C-70142
2-Chloro-5-phenylpyrazine, C-70143
2-Chloro-6-phenylpyrazine, C-70144
2-Chloro-4-phenylpyrimidine, C-80100
4-Chloro-2-phenylpyrimidine, C-80102
4-Chloro-5-phenylpyrimidine, C-80103
4-Chloro-6-phenylpyrimidine, C-80104
5-Chloro-2-phenylpyrimidine, C-80105
5-Chloro-4-phenylpyrimidine, C-80106

$C_{10}H_7ClN_2O$
2-Chloro-3-phenylpyrazine; 1-Oxide, *in* C-70142
2-Chloro-3-phenylpyrazine; 4-Oxide, *in* C-70142
2-Chloro-5-phenylpyrazine; 1-Oxide, *in* C-70143
2-Chloro-5-phenylpyrazine; 4-Oxide, *in* C-70143
2-Chloro-6-phenylpyrazine; 1-Oxide, *in* C-70144
2-Chloro-6-phenylpyrazine; 4-Oxide, *in* C-70144

$C_{10}H_7ClN_2O_2$
2-Chloro-3-phenylpyrazine; 1,4-Dioxide, *in* C-70142
2-Chloro-5-phenylpyrazine; 1,4-Dioxide, *in* C-70143

$C_{10}H_7ClO_3$
4-Hydroxy-5-benzofurancarboxylic acid; Me ether, chloride, *in* H-60103

$C_{10}H_7ClO_4$
6-Chloro-1,2,3,4-naphthalenetetrol, C-60118

$C_{10}H_7Cl_2NO_2$
5,6-Dichloro-1*H*-indole-3-acetic acid, D-70123

$C_{10}H_7F_5O_2$
Pentafluorophenylacetic acid; Et ester, *in* P-80027

$C_{10}H_7N$
2-Ethynylindole, E-60057
3-Ethynylindole, E-60058
4-Ethynylindole, E-80074

$C_{10}H_7NOS$
3-Phenyl-2-propenoyl isothiocyanate, P-70090

$C_{10}H_7NO_2$
3-Benzoylisoxazole, B-70075
4-Benzoylisoxazole, B-60062
5-Benzoylisoxazole, B-60063

$C_{10}H_7NO_2S$
2-Amino-3-mercapto-1,4-naphthoquinone, A-70163

$C_{10}H_7NO_3$
3-Hydroxy-2-quinolinecarboxylic acid, H-60228
2-Phenyl-4-oxazolecarboxylic acid, P-80109
2-Phenyl-5-oxazolecarboxylic acid, P-80110
5-Phenyl-2-oxazolecarboxylic acid, P-80111
5-Phenyl-4-oxazolecarboxylic acid, P-80112

$C_{10}H_7NO_4$
1-Nitro-2,6-naphthalenediol, N-80048
2-Nitro-1,4-naphthalenediol, N-80050
2-Nitro-1,5-naphthalenediol, N-80051
2-Nitro-1,7-naphthalenediol, N-80052
4-Nitro-1,2-naphthalenediol, N-80053
4-Nitro-1,5-naphthalenediol, N-80054
4-Nitro-1,7-naphthalenediol, N-80055
6-Nitro-2,3-naphthalenediol, N-80056
2-Oxo-3-indolineglyoxylic acid, O-80085

$C_{10}H_7NS$
2-(1,2-Propadienyl)benzothiazole, P-60174

$C_{10}H_7N_3$
1*H*-Imidazo[4,5-*f*]quinoline, I-70007
1*H*-Imidazo[4,5-*h*]quinoline, I-70008
Pyrazolo[3,4-*c*]quinoline, P-60206
1*H*-Pyrido[3,4,5-*de*]quinazoline, P-80217
1*H*-Pyrido[4,3,2-*de*]quinazoline, P-80218

$C_{10}H_7N_3O$
2,5-Dihydro-1*H*-dipyrido[4,3-*b*:3′,4′-*d*]pyrrol-1-one, D-60237
3,5-Dihydro-4*H*-pyrazolo[3,4-*c*]quinolin-4-one, D-80245

$C_{10}H_8$
Fulvalene, F-60080
Naphthvalene, N-60012
Tetracyclo[5.3.0.0^{2,4}.0^{3,5}]deca-6,8,10-triene, T-70019

$C_{10}H_8BrN$
3-Bromo-5-methylisoquinoline, B-80218
4-Bromo-1-methylisoquinoline, B-80219
5-Bromo-3-methylisoquinoline, B-80220

$C_{10}H_8ClN$
2-Chloro-1-naphthylamine, C-80080

$C_{10}H_8ClNO_4$
2[(Chlorocarbonyl)oxy]-3*a*,4,7,7*a*-tetrahydro-4,7-methano-1*H*-isoindole-1,3(2*H*)-dione, C-70059

$C_{10}H_8ClN_3O_4$
Pyrido[1′,2′:3,4]imidazo[1,2-*a*]pyrimidin-5-ium(1+); Perchlorate, *in* P-70176

$C_{10}H_8FN$
2-Fluoro-4-methylquinoline, F-80050
3-Fluoro-4-methylquinoline, F-80051
4-Fluoro-2-methylquinoline, F-80052
6-Fluoro-2-methylquinoline, F-80053
6-Fluoro-5-methylquinoline, F-80054
7-Fluoro-2-methylquinoline, F-80055

$C_{10}H_8N_2$
▷ 2,3′-Bipyridine, B-60120
2,4′-Bipyridine, B-60121
3,3′-Bipyridine, B-60122
3,4′-Bipyridine, B-60123
1,8-Dihydrobenzo[2,1-*b*:3,4-*b*′]dipyrrole, D-70174
5-Phenylpyrimidine, P-70093
▷ 1*H*-*Indole*-3-*acetonitrile*, *in* I-70013

$C_{10}H_8N_2O$
2-Acetylquinoxaline, A-60056
5-Acetylquinoxaline, A-60057
6-Acetylquinoxaline, A-60058
2-Benzoylimidazole, B-70074
4(5)-Benzoylimidazole, B-60057
3-Benzoylpyrazole, B-70078
4-Benzoylpyrazole, B-60065
3,3′-Bipyridine; Mono-*N*-oxide, *in* B-60122
2,3′-Bipyridine; 1′-Oxide, *in* B-60120
2,4′-Bipyridine; 1-Oxide, *in* B-60121
4,6-Dihydroxy-2,2′-bipyridine, D-80296
2′-Hydroxy-2,3′-bipyridine, H-80117
2′-Hydroxy-2,4′-bipyridine, H-80118
2-Hydroxy-3,3′-bipyridine, H-80119
2-Hydroxy-4,4′-bipyridine, H-80120
4-Hydroxy-2,2′-bipyridine, H-80121
4-Hydroxy-3,3′-bipyridine, H-80122
5-Hydroxy-2,2′-bipyridine, H-80123
5-Hydroxy-2,3′-bipyridine, H-80124
5-Hydroxy-3,3′-bipyridine, H-80125
6-Hydroxy-2,2′-bipyridine, H-80126
6-Hydroxy-2,3′-bipyridine, H-80127
6-Hydroxy-2,4′-bipyridine, H-80128
6-Hydroxy-3,3′-bipyridine, H-80129
6-Hydroxy-3,4′-bipyridine, H-80130
2,2′-Oxybispyridine, O-60098
2,3′-Oxybispyridine, O-60099
2,4′-Oxybispyridine, O-80099
3,3′-Oxybispyridine, O-60100
3,4′-Oxybispyridine, O-80100
4,4′-Oxybispyridine, O-60101
2-Phenyl-1*H*-imidazole-4(5)-carboxaldehyde, P-60111
3-Phenyl-4(1*H*)-pyridazinone, P-80124
5-Phenylpyrimidine; *N*-Oxide, *in* P-70093
1*H*-Pyrazole; *N*-Benzoyl, *in* P-70152
1-(2-Pyridyl)-2-pyridone, P-80219
1-(2-Pyridyl)-4-pyridone, P-80220
1-(3-Pyridyl)-4-pyridone, P-80221
1-(4-Pyridyl)-2-pyridone, P-80222
1-(4-Pyridyl)-4-pyridone, P-80223

$C_{10}H_8N_2OS$
2,3-Dihydro-6-phenyl-2-thioxo-4(1*H*)-pyrimidinone, D-60268

$C_{10}H_8N_2O_2$
5-Amino-3-phenylisoxazole; *N*-Formyl, *in* A-60240
4-Benzoylisoxazole; Oxime, *in* B-60062
2,3′-Bipyridine; 1,1′-Dioxide, *in* B-60120
2,4′-Bipyridine; 1,1′-Dioxide, *in* B-60121
2,2′-Dihydroxy-3,3′-bipyridine, D-80287
2,2′-Dihydroxy-4,4′-bipyridine, D-80288
2,4′-Dihydroxy-1,1′-bipyridine, D-80289
3,3′-Dihydroxy-2,2′-bipyridine, D-80290
3,3′-Dihydroxy-4,4′-bipyridine, D-80291
3,4′-Dihydroxy-2,3′-bipyridine, D-80292
4,4′-Dihydroxy-1,1′-bipyridine, D-80293
4,4′-Dihydroxy-2,2′-bipyridine, D-80294
4,4′-Dihydroxy-3,3′-bipyridine, D-80295
5,5′-Dihydroxy-2,2′-bipyridine, D-80297
5,5′-Dihydroxy-3,3′-bipyridine, D-80298
6,6′-Dihydroxy-2,2′-bipyridine, D-80299
6,6′-Dihydroxy-3,3′-bipyridine, D-80300
3-Hydroxy-2-quinolinecarboxylic acid; Amide, *in* H-60228
3,3′-Oxybispyridine; *N*-Oxide, *in* O-60100

$C_{10}H_8N_2O_2S$
▷ 2-Thioxo-4-imidazolidinone; 1-*N*-Benzoyl, *in* T-70188

$C_{10}H_8N_2O_2S_2Zn$
▷ Bis(1-hydroxy-2(1*H*)-pyridinethionato-*O*,*S*)zinc, *in* P-60224

$C_{10}H_8N_2O_3$
2-Acetylquinoxaline; 1,4-Dioxide, *in* A-60056
3,3′-Oxybispyridine; *N*,*N*′-Dioxide, *in* O-60100

$C_{10}H_8N_2O_3S$
Di-2-pyridyl sulfite, D-60497

$C_{10}H_8N_2O_4$
4,4′-Dihydroxy-2,2′-bipyridine; 1,1′-Dioxide, *in* D-80294

$C_{10}H_8N_2O_8$
4,6-Dinitro-1,3-benzenediol; Di-Ac, *in* D-80491

$C_{10}H_8N_2S$
2,3′-Thiobispyridine, T-80186
2,4′-Thiobispyridine, T-80187
3,4′-Thiobispyridine, T-80188

$C_{10}H_8N_2Se$
2,2′-Selenobispyridine, S-80023

$C_{10}H_8N_3^{\oplus}$
Pyrido[1′,2′:3,4]imidazo[1,2-*a*]pyrimidin-5-ium(1+), P-70176

$C_{10}H_8N_4$
4-Amino-1*H*-1,5-benzodiazepine-3-carbonitrile, A-70091
5-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Ph, nitrile, *in* A-70192
Dipyrido[1,2-*b*:1′,2′-*e*][1,2,4,5]tetrazine, D-60494

$C_{10}H_8O$
2,8-Decadiene-4,6-diyn-1-al, D-80008
▷ 3-Phenyl-2-cyclobuten-1-one, P-70064

$C_{10}H_8OS$
1-Benzothiepin-5(4*H*)-one, B-60047

$C_{10}H_8O_2$
1,2-Di(2-furanyl)ethylene, D-60191
4-Hydroxy-1-phenyl-2-butyn-1-one, H-80233
6-Hydroxy-5-vinylbenzofuran, H-70231
3-Methyl-1*H*-2-benzopyran-1-one, M-70052
2-(3-Oxo-1-propenyl)benzaldehyde, O-60091
3-Phenyl-2(5*H*)furanone, P-60102
4-Phenyl-2(5*H*)-furanone, P-60103
5-Phenyl-2(3*H*)-furanone, P-70079

$C_{10}H_8O_2S$
5-[(5-Methyl-2-thienyl)methylene]-2(5*H*)-furanone, M-80161
5-(5-Methyl-2-thienyl)-2-penten-4-ynoic acid, M-80162
5-(2-Thienyl)-2-penten-4-ynoic acid; Me ester, *in* T-80183

$C_{10}H_8O_3$
3-Benzofurancarboxylic acid; Me ester, *in* B-60032
4,6-Dihydroxy-5-vinylbenzofuran, D-70352
5-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one, H-60173
8-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one, H-70165
6-Methoxy-2*H*-1-benzopyran-2-one, *in* H-70109
1,4,5-Naphthalenetriol, N-60005

$C_{10}H_8O_3S$
2-Oxo-4-phenylthio-3-butenoic acid, O-60088

$C_{10}H_8O_4$
Albidin, A-60070
4,7-Dihydroxy-5-methyl-2*H*-1-benzopyran-2-one, D-60348
3,4-Dimethoxbenzocyclobutene-1,2-dione, *in* D-80274
3,5-Dimethoxybenzocyclobutene-1,2-dione, *in* D-80275
3,6-Dimethoxybenzocyclobutene-1,2-dione, *in* D-80276
4,5-Dimethoxybenzocyclobutene-1,2-dione, *in* D-80277
4-Hydroxy-5-benzofurancarboxylic acid; Me ester, *in* H-60103
5-Hydroxy-3(2*H*)-benzofuranone; Ac, *in* H-80109
6-Hydroxy-3(2*H*)-benzofuranone; Ac, *in* H-80110
7-Hydroxy-6-(hydroxymethyl)-2*H*-1-benzopyran-2-one, H-70139
5-Hydroxy-4-(4-hydroxyphenyl)-2(5*H*)-furanone, H-80174
6-Hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, H-80188
▷ 7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, H-80189
4-Methoxy-5-benzofurancarboxylic acid, *in* H-60103
1,4,5,7-Naphthalenetetrol, N-80003

$C_{10}H_8O_4Se_2$
1,8-Naphthalenediseleninic acid, N-80002

$C_{10}H_8O_5$
5,6-Dihydroxy-7-methoxy-2*H*-1-benzopyran-2-one, *in* T-80287
2-Hydroxy-4,5-methylenedioxybenzaldehyde; Ac, *in* H-70175

$C_{10}H_8O_6$
2-Acetoxy-1,3-benzenedicarboxylic acid, *in* H-60101
1,4-Benzoquinone-2,3-dicarboxylic acid; Di-Me ester, *in* B-70047
1,4-Benzoquinone-2,5-dicarboxylic acid; Di-Me ester, *in* B-70048

$C_{10}H_8S_2$
1,2-Naphthalenedithiol, N-70002
1,8-Naphthalenedithiol, N-70003
2,3-Naphthalenedithiol, N-70004

$C_{10}H_8S_8$
2-(5,6-Dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-ylidene)-5,6-dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin, D-60238

$C_{10}H_9Br$
3-Bromo-1-phenyl-1-butyne, B-60314

$C_{10}H_9BrN_2$
4(5)-Bromo-1*H*-imidazole; 1-Benzyl, *in* B-70221

$C_{10}H_9BrO$
7-Bromo-3,4-dihydro-1(2*H*)-naphthalenone, B-60234

$C_{10}H_9ClN_2$
1-Benzyl-3-chloropyrazole, *in* C-70155
1-Benzyl-5-chloropyrazole, *in* C-70155

$C_{10}H_9IO_2$
1,3-Diacetyl-5-iodobenzene, D-60024

$C_{10}H_9N$
2-Vinylindole, V-70013

$C_{10}H_9NO$
2-Acetylindole, A-60032
4-Acetylindole, A-60033
▷ 5-Acetylindole, A-60034
6-Acetylindole, A-60035
7-Acetylindole, A-60036
1,2-Dihydro-1-phenyl-3*H*-pyrrol-3-one, *in* D-70262
1-(2-Furanyl)-2-(2-pyrrolyl)ethylene, F-60088
1-(4-Hydroxyphenyl)pyrrole, H-60216
2-(2-Hydroxyphenyl)pyrrole, H-60217
6-Methoxyisoquinoline, *in* H-80178
3-Methyl-1*H*-indole-2-carboxaldehyde, M-70090
2-Methyl-5-phenyloxazole, M-80145

$C_{10}H_9NOS$
1,4-Benzothiazepin-5(4*H*)-one; *N*-Me, *in* B-80040

$C_{10}H_9NO_2$
2-Acetyl-3-aminobenzofuran, A-70021
1-Amino-2,6-naphthalenediol, A-80112
1-Amino-2,7-naphthalenediol, A-80113
2-Amino-1,4-naphthalenediol, A-80114
2-Amino-1,6-naphthalenediol, A-80115
3-Amino-1,2-naphthalenediol, A-80116
4-Amino-1,2-naphthalenediol, A-80117
4-Amino-1,3-naphthalenediol, A-80118
4-Amino-1,5-naphthalenediol, A-80119
4-Amino-1,7-naphthalenediol, A-80120
5-Amino-1,2-naphthalenediol, A-80121
5-Amino-2,3-naphthalenediol, A-80122
6-Amino-2,3-naphthalenediol, A-80123
6-Amino-1,2-napthalenediol, A-80124
3-Azetidinone; 1-Benzoyl, *in* A-80192
6-Hydroxyisoquinoline; Me ether, *N*-oxide, *in* H-80178
4-Hydroxy-5-nitro-1,2-benzenedicarboxylic acid; Di-Me ester, *in* H-70191
▷ 1*H*-Indole-3-acetic acid, I-70013
1*H*-Indole-3-carboxylic acid; Me ester, *in* I-80012
1*H*-Indole-3-carboxylic acid; N-Me, *in* I-80012
Phthalimidine; *N*-Ac, *in* P-70100

$C_{10}H_9NO_2S$
α-Aminobenzo[*b*]thiophene-3-acetic acid, A-60090
3-Amino-2-benzo[*b*]thiophenecarboxylic acid; Me ester, *in* A-60091

$C_{10}H_9NO_2S_2$
N-Phenyl-2-thiophenesulfonamide, *in* T-60213
N-Phenyl-3-thiophenesulfonamide, *in* T-60214

$C_{10}H_9NO_3$
2,3-Dihydro-2-oxo-1*H*-indole-3-acetic acid, D-60259
2-Nitro-3,4-dihydro-1(2*H*)naphthalenone, N-60026
1,2,3,4-Tetrahydro-2-oxo-4-quinolinecarboxylic acid, T-60077
1,2,3,4-Tetrahydro-4-oxo-6-quinolinecarboxylic acid, T-60078
1,2,3,4-Tetrahydro-4-oxo-7-quinolinecarboxylic acid, T-60079

$C_{10}H_9NO_6$
2-Nitro-1,3-benzenedicarboxylic acid; Di-Me ester, *in* N-80035

$C_{10}H_9NO_7$
4-Hydroxy-5-nitro-1,3-benzenedicarboxylic acid; Di-Me ester, *in* H-70192
4-Hydroxy-3-nitro-1,2-benzenedicarboxylic acid; Me ether, 2-Me ester, *in* H-70190

$C_{10}H_9NS$
1-Amino-2-naphthalenethiol, A-70172
8-Amino-1-naphthalenethiol, A-70173
3(2*H*)-Isoquinolinethione; *S*-Me; B,HCl, *in* I-60133
1-Methylthioisoquinoline, *in* I-60132
4-Methylthioquinoline, *in* Q-60006
5-Methylthioquinoline, *in* Q-60004
6-Methylthioquinoline, *in* Q-60005
1-(2-Pyrrolyl)-2-(2-thienyl)ethylene, P-60250
3-Quinolinethiol; *S*-Me, *in* Q-60003
4(1*H*)-Quinolinethione; *N*-Me, *in* Q-60006

$C_{10}H_9NS_2$
2-Thiazoledinethione; *N*-Ph, *in* T-60197

$C_{10}H_9N_3$
6-Methyl-3-phenyl-1,2,4-triazine, M-60118
3-(Phenylazo)-2-butenenitrile, P-60079

$C_{10}H_9N_3O$
1-Acetamidophthalazine, *in* A-70184
2-Acetylquinoxaline; Oxime, *in* A-60056
4-Benzoyl-1,2,3-triazole; 1-Me, *in* B-70079
4-Benzoyl-1,2,3-triazole; 2-Me, *in* B-70079
4-Benzoyl-1,2,3-triazole; 3-Me, *in* B-70079

$C_{10}H_9N_3O_2$
4-Amino-1*H*-pyrazole-3-carboxylic acid; 1-Ph, *in* A-70189
2-Phenyl-2*H*-1,2,3-triazole-4-carboxylic acid; Me ester, *in* P-60140

$C_{10}H_9N_3O_9$
3-Hydroxy-5-methyl-2,4,6-trinitrobenzoic acid; Me ether, Me ester, *in* H-60193

$C_{10}H_{10}$
Bi-2,4-cyclopentadien-1-yl, B-60100
3-Cyclodecene-1,5-diyne, C-80177
7,8-Dimethylenebicyclo[2.2.2]octa-2,5-diene, D-70407
Hexacyclo[4.4.0.0^{2,5}.0^{3,9}.O^{4,8}.0^{7,10}]decane, H-70032
9-Methylene-1,3,5,7-cyclononatetraene, M-60073
1-Methyleneindane, M-60078
1,4,5,6-Tetrahydrocycloprop[*e*]indene, T-70053
1,3,4,5-Tetrahydrocycloprop[*f*]indene, T-70052
1,3,4,5-Tetrahydrocycloprop[*f*]indene, T-80056
Tricyclo[5.3.0.0^{2,8}]deca-3,5,9-triene, T-70227

$C_{10}H_{10}N_2$
1-Amino-3-methylisoquinoline, A-80098
3-Amino-1-methylisoquinoline, A-80099
3-Amino-4-methylisoquinoline, A-80100
4-Amino-1-methylisoquinoline, A-80101
5-Amino-1-methylisoquinoline, A-80102
7-Amino-1-methylisoquinoline, A-80104
8-Amino-1-methylisoquinoline, A-80105
1,8-Diaminonaphthalene, D-70042
1,4-Dihydro-2-phenylpyrimidine, D-70249

$C_{10}H_{10}N_2O$
5-Acetylindole; Oxime, *in* A-60034
5-Amino-3-phenylisoxazole; *N*-Me, *in* A-60240
5,6-Dihydro-2-phenyl-4(1*H*)-pyrimidinone, D-70250
1*H*-Indole-3-acetic acid; Amide, *in* I-70013

$C_{10}H_{10}N_2O_2$
1,2-Diazetidin-3-one; 1-Ac, 2-Ph, *in* D-70055
5,6-Dihydro-6-phenyl-2,4(1*H*, 3*H*)-pyrimidinedione, D-80240
1,4-Dihydro-2,3-quinoxalinedione; 1,4-Di-Me, *in* D-60279
2,3-Dimethoxyquinoxaline, *in* D-60279
5,8-Dimethoxyquinoxaline, *in* Q-60002
6,7-Dimethoxyquinoxaline, *in* Q-60009
3-Ethoxy-2-quinoxalinol, *in* D-60279
3-Ethoxy-2(1*H*)quinoxalinone, *in* D-60279
5,8-Quinoxalinediol; Di-Me ether, *in* Q-60008

$C_{10}H_{10}N_2O_4$
1,4-Dihydropyrrolo[3,2-*b*]pyrrole; 1,4-Bis(methoxycarbonyl), *in* D-30286

$C_{10}H_{10}N_2O_6$
3-Amino-4-nitro-1,2-benzenedicarboxylic acid; Di-Me ester, *in* A-70174
3-Amino-6-nitro-1,2-benzenedicarboxylic acid; Di-Me ester, *in* A-70175
4-Amino-3-nitro-1,2-benzenedicarboxylic acid; Di-Me ester, *in* A-70176

$C_{10}H_{10}N_4$
2-Hydroxy-4,4′-bipyridine; Hydrazone, *in* H-80120

$C_{10}H_{10}N_4O$
3-Amino-1*H*-pyrazole-4-carboxylic acid; Anilide, *in* A-70187
4-Amino-1*H*-pyrazole-3-carboxylic acid; 1-Ph, amide, *in* A-70189
5-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Ph, amide, *in* A-70192

$C_{10}H_{10}O$
2,3-Dihydro-6(1*H*)-azulenone, D-60193
4,7-Dihydro-4,7-ethanoisobenzofuran, D-60240
2-Methyl-1-phenyl-2-propen-1-one, M-80146
Pentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decan-6-one, P-60027
1-Phenyl-3-buten-1-one, P-60085
1-Phenyl-2-butyn-1-ol, P-70062
4-Phenyl-3-butyn-2-ol, P-70063
2-(2-Propenyl)benzaldehyde, P-70122
4-(2-Propenyl)benzaldehyde, P-60177
[3](2,7)Troponophane, T-70329

$C_{10}H_{10}OS$
1-Methylene-2-(phenylsulfinyl)cyclopropane, *in* M-80090

$C_{10}H_{10}O_2$
2-Benzoylpropanal, B-80057
1,3,5,7-Cyclooctatetraene-1-acetic acid, C-70237
Cyclooctatetraenecarboxylic acid; Me ester, *in* C-70239
2,5,8-Decatriyne-1,10-diol, D-80016
8-Decene-4,6-diynoic acid, D-70018
3*a*,6*a*-Dihydro-3*a*,6*a*-dimethyl-1,6-pentalenedione, D-70199
Dihydro-5-phenyl-2(3*H*)-furanone, D-80239
2,3-Dimethyl-1,4-benzodioxin, D-70370
3,3-Dimethyl-2(3*H*)-benzofuranone, D-80418
4,9-Dioxa-1,6,11-dodecatriyne, D-80499
11,12-Dioxahexacyclo[6.2.1.1^{3,6}.0^{2,7}.0^{4,10}.0^{5,9}]dodecane, D-70461
5,12-Dioxatetracyclo[7.2.1.0^{4,11}.0^{6,10}]dodeca-2,7-diene, D-70463
Dispiro[2.0.2.4]dec-8-ene-7,10-dione, D-60501
(4-Hydroxyphenyl)ethylene; Ac, *in* H-70209
Isosafrole, I-80089
3-(4-Methoxyphenyl)-2-propenal, *in* H-60213
2-Phenyl-3-butenoic acid, P-80096
2-Phenylcyclopropanecarboxylic acid, P-60087
5,6,7,8-Tetrahydro-1,4-naphthoquinone, T-80076

$C_{10}H_{10}O_2S$
2-Acetyl-3-methoxy-5-(1-propynyl)thiophene, *in* A-80024
4′-Mercaptoacetophenone; Ac, *in* M-60017
1-Methylene-2-(phenylsulfonyl)cyclopropane, *in* M-80090
S-Phenyl 3-oxobutanethioate, *in* O-70080
2-Phenylsulfonyl-1,3-butadiene, P-70094

$C_{10}H_{10}O_2S_2$
2,3,8,9-Tetrahydrobenzo[2,1-*b*:3,4-*b*′]bis[1,4]oxathiin, T-70040

$C_{10}H_{10}O_3$
2-Acetylbenzoic acid; Me ester, *in* A-80015
5-Acetyl-2-methoxybenzaldehyde, *in* A-80022
Coniferaldehyde, C-80148
3,4-Dihydro-4,8-dihydroxy-1(2*H*)-naphthalenone, D-80181
3,6-Dimethoxybenzocyclobuten-1-one, *in* D-80278
4,5-Dimethoxybenzocyclobuten-1-one, *in* D-80279

4,6-Dimethoxybenzocyclobuten-1-one, *in* D-80280
5,6-Dimethoxybenzocyclobuten-1-one, *in* D-80281
4-Ethoxy-3(2*H*)-benzofuranone, *in* H-80108
Hexahydrocyclopenta[*cd*]pentalene-1,3,5(2*H*)-trione, H-60048
8-Hydroxy-2-decene-4,6-diynoic acid, H-80150
2-Hydroxy-2-phenylacetaldehyde; Ac, *in* H-60210
3-(4-Hydroxyphenyl)-2-propenoic acid; Me ester, *in* H-80242
3-(4-Methoxyphenyl)-2-propenoic acid, *in* H-80242
3-Oxopropanoic acid; Benzyl ester, *in* O-60090

$C_{10}H_{10}O_3S$
2-Mercaptopropanoic acid; *S*-Benzoyl, *in* M-60027

$C_{10}H_{10}O_4$
1,4-Benzodioxan-2-carboxylic acid; Me ester, *in* B-60024
1,4-Benzodioxan-6-carboxylic acid; Me ester, *in* B-60025
4*H*-1,3-Benzodioxin-6-carboxylic acid; Me ester, *in* B-60027
1,3,5-Cycloheptatriene-1,6-dicarboxylic acid; Mono-Me ester, *in* C-60202
3,4-Dihydroxyphenylacetaldehyde; 3-Me ether, Ac, *in* D-60371
5,7-Dimethoxyphthalide, *in* D-60339
5-Hydroxy-7-methoxy-6-methylphthalide, *in* D-60349
2-Hydroxy-4-methylbenzoic acid; Ac, *in* H-70163
Mesogentiogenin, *in* G-80009
1-(2,4,6-Trihydroxyphenyl)-2-buten-1-one, T-80331

$C_{10}H_{10}O_5$
2,3-Dihydroxy-5-methyl-1,4-benzoquinone; 2-Me ether, 3-Ac, *in* D-70320
2,3-Dihydroxy-5-methyl-1,4-benzoquinone; 3-Me ether, 2-Ac, *in* D-70320
2-Formyl-3,4-dimethoxybenzoic acid, *in* F-60070
4-Formyl-2,5-dimethoxybenzoic acid, *in* F-60072
6-Formyl-2,3-dimethoxybenzoic acid, *in* F-60073
2-Hydroxy-1,3-benzenedicarboxylic acid; Di-Me ester, *in* H-60101
2-Hydroxy-1,4-benzenedicarboxylic acid; Di-Me ester, *in* H-70105
5-Hydroxy-3-methyl-1,2-benzenedicarboxylic acid; Me ether, *in* H-70162
2-Hydroxy-3,4-methylenedioxybenzoic acid; Me ether, Me ester, *in* H-60177
3-Hydroxy-4,5-methylenedioxybenzoic acid; Me ether, Me ester, *in* H-60178
4-Hydroxy-2,3-methylenedioxybenzoic acid; Me ether, Me ester, *in* H-60179
(2-Hydroxyphenoxy)acetic acid; *O*-Ac, *in* H-70203

$C_{10}H_{10}O_6$
Chorismic acid, C-70173
4,5-Dihydroxy-1,3-benzenedicarboxylic acid; Di-Me ester, *in* D-60307
4,5-Dimethoxy-1,3-benzenedicarboxylic acid, *in* D-60307

$C_{10}H_{10}S$
3-Methyl-2*H*-1-benzothiopyran, M-80051
1-Methylene-2-(phenylthio)cyclopropane, M-80090

$C_{10}H_{10}S_2$
2,2′-Dimethyl-3,3′-bithiophene, D-80430
3,3′-Dimethyl-2,2′-bithiophene, D-80431
3,4′-Dimethyl-2,2′-bithiophene, D-80432
3,5-Dimethyl-2,3′-bithiophene, D-80433
4,4′-Dimethyl-2,2′-bithiophene, D-80434
4,4′-Dimethyl-3,3′-bithiophene, D-80435
5,5′-Dimethyl-2,2′-bithiophene, D-80436
5,5′-Dimethyl-3,3′-bithiophene, D-80437

$C_{10}H_{10}S_4$
2,3,8,9-Tetrahydrobenzo[1,2-*b*:3,4-*b*′]bis[1,4]dithiin, T-70039

$C_{10}H_{11}Br$
1-Bromo-2-methyl-1-phenylpropene, B-80228

$C_{10}H_{11}BrN_4O_5$
2-Bromo-9-β-D-ribofuranosyl-6*H*-purin-6-one, B-70269
8-Bromo-9-β-D-ribofuranosyl-6*H*-purin-6-one, B-70270

$C_{10}H_{11}BrO_2$
2-Bromo-4-phenylbutanoic acid, B-80242
3-Bromo-2,4,6-trimethylbenzoic acid, B-60331

$C_{10}H_{11}ClN_4O_4$
2-Chloro-9-β-D-ribofuranosyl-9*H*-purine, C-70159
6-Chloro-9-β-D-ribofuranosyl-9*H*-purine, C-70160

$C_{10}H_{11}ClN_4O_5$
2-Chloro-9-β-D-ribofuranosyl-6*H*-purin-6-one, C-70161

$C_{10}H_{11}ClO_2$
2-Chloro-1-phenylethanol; Ac, *in* C-80099
2-Chloro-2-phenylethanol; Ac, *in* C-60128

$C_{10}H_{11}ClO_3$
5-Chloro-4-hydroxy-2-methylbenzoic acid; Me ether, Me ester, *in* C-60097

$C_{10}H_{11}F$
4-Fluoro-1-phenyl-1-butene, F-70035

$C_{10}H_{11}FO_4$
Methyl 4-fluoro-3,5-dimethoxybenzoate, *in* F-60024

$C_{10}H_{11}IO$
2-Iodo-1-phenyl-1-butanone, I-60060

$C_{10}H_{11}IO_4$
2,3-Dihydroxy-6-iodobenzoic acid; Di-Me ether, Me ester, *in* D-60330
2,4-Dihydroxy-5-iodobenzoic acid; Di-Me ether, Me ester, *in* D-60332
2,6-Dihydroxy-3-iodobenzoic acid; Di-Me ether, Me ester, *in* D-60334
3,4-Dihydroxy-5-iodobenzoic acid; Di-Me ether, Me ester, *in* D-60335
Methyl 2-iodo-3,5-dimethoxybenzoate, *in* D-60336
Methyl 4-iodo-3,5-dimethoxybenzoate, *in* D-60337

$C_{10}H_{11}N$
1-Amino-1,4-dihydronaphthalene, A-60139
1-Amino-5,8-dihydronaphthalene, A-60140
3,4-Dihydro-5-phenyl-2*H*-pyrrole, D-70251
1,6-Dimethyl-1*H*-indole, *in* M-60088
2,2-Dimethyl-3-phenyl-2*H*-azirine, D-60440
2-(4-Methylphenyl)propanoic acid; Nitrile, *in* M-60114

$C_{10}H_{11}NO$
3-Ethoxy-1*H*-isoindole, *in* P-70100
Phthalimidine; *N*-Et, *in* P-70100

$C_{10}H_{11}NOS$
4-Methyl-5-phenyl-2-oxazolidinethione, M-60111
Tetrahydro-2-phenyl-2*H*-1,2-thiazin-3-one, *in* T-60095

$C_{10}H_{11}NO_2$
2-Amino-3-phenyl-3-butenoic acid, A-60238
2-Amino-4-phenyl-3-butenoic acid, A-60239
5,6-Dimethoxyindole, *in* D-70307
5-Methyl-3-phenyl-2-oxazolidinone, *in* M-60107
4-Phenyl-3-morpholinone, *in* M-60147
1,2,3,4-Tetrahydro-1-isoquinolinecarboxylic acid, T-60070
5,6,7,8-Tetrahydro-1,4-naphthoquinone; Monoxime, *in* T-80076

$C_{10}H_{11}NO_2S$
3,4-Dimethoxybenzyl isothiocyanate, D-80411

$C_{10}H_{11}NO_3$
1-Amino-2-(4-hydroxyphenyl)cyclopropanecarboxylic acid, A-60197
3-Amino-4-oxo-4-phenylbutanoic acid, A-60236
4-Hydroxyphenylacetaldehyde; Ac, oxime, *in* H-60209
Methyl *N*-phenacylcarbamate, *in* O-70099
2,3,5-Trimethoxybenzonitrile, *in* T-70250

$C_{10}H_{11}NO_4$
3-Amino-2-hydroxypropanoic acid; Benzoyl, *in* A-70160
2,3,4-Trimethyl-5-nitrobenzoic acid, T-60369
2,4,6-Trimethyl-3-nitrobenzoic acid, T-60370

$C_{10}H_{11}NO_4S$
2,3-Dihydro-1*H*-indole-2-sulfonic acid; *N*-Ac, *in* D-70221

$C_{10}H_{11}NO_5$
4-Amino-6-hydroxy-1,3-benzenedicarboxylic acid; Di-Me ester, *in* A-70153
5-Amino-2-hydroxy-1,3-benzenedicarboxylic acid; Di-Me ester, *in* A-70154
5-Amino-4-hydroxy-1,3-benzenedicarboxylic acid; Di-Me ester, *in* A-70155
2′,3′-Dimethoxy-6′-nitroacetophenone, *in* D-60357
2′,5′-Dimethoxy-4′-nitroacetophenone, *in* D-70322
3′,6′-Dimethoxy-2′-nitroacetophenone, *in* D-60358
4′,5′-Dimethoxy-2′-nitroacetophenone, *in* D-60359

$C_{10}H_{11}N_3$
1-Aminophthalazine; *N*,*N*-Di-Me, *in* A-70184
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid; 1-Me, dinitrile, *in* D-80193
2-(3,5-Dimethyl-1*H*-pyrazol-1-yl)pyridine, D-80473

$C_{10}H_{11}N_3O$
3,4-Diamino-1-methoxyisoquinoline, D-60037
▷ 1*H*-Indole-3-acetic acid; Hydrazide, *in* I-70013

$C_{10}H_{11}N_5$
2,4-Diamino-6-methyl-1,3,5-triazine; *N*-Ph, *in* D-60040

$C_{10}H_{11}N_5O$
1,4-Dihydro-4,6,7-trimethyl-9*H*-imidazo[1,2-*a*]purin-9-one, D-70278

$C_{10}H_{11}N_5O_3$
6-Amino-1,3-dihydro-2*H*-purin-2-one; 6,9-Di-Ac, 1-Me, *in* A-60144

$C_{10}H_{12}$
1,3,5,7,9-Decapentaene, D-70015
5-Decene-2,8-diyne, D-60015
[4]Metacyclophane, M-60029
[4]Paracyclophane, P-60006
4,5,6,7-Tetrahydro-1-methylene-1*H*-indene, T-70073
Tricyclo[4.2.2.0^{1,6}]deca-7,9-diene, T-70226
2,3,5-Tris(methylene)bicyclo[2.2.1]heptane, T-60403

$C_{10}H_{12}BrNO$
2-Bromo-2-methylpropanoic acid; Anilide, *in* B-80229
2-Bromo-4-phenylbutanoic acid; Amide, *in* B-80242

$C_{10}H_{12}BrN_5O_5$
8-Bromoguanosine, B-70215

$C_{10}H_{12}ClN_5O_5$
8-Chloroguanosine, C-70068

$C_{10}H_{12}FN_5O_4$
8-Amino-6-fluoro-9*H*-purine; 9-β-D-Ribofuranosyl, *in* A-60163

$C_{10}H_{12}IN_5O_5$
8-Iodoguanosine, I-70034

$C_{10}H_{12}N_2O$
4-Imidazolidinone; 3-Benzyl, *in* I-80006
1-Phenyl-2-piperazinone, *in* P-70101

$C_{10}H_{12}N_2O_3$
3-Amino-4(1*H*)-pyridinone; 1-*N*-Me, N^3,N^3-di-Ac, *in* A-60254

$C_{10}H_{12}N_2O_4$
3,6-Pyridazinedicarboxylic acid; Di-Et ester, *in* P-70168
10,11,14,15-Tetraoxa-1,8-diazatricyclo[6.4.4.0^{2,7}]hexadeca-2(7),3,5-triene, T-60162

$C_{10}H_{12}N_2O_6$
1,5-Diethoxy-2,4-dinitrobenzene, *in* D-80491

$C_{10}H_{12}N_2S$
2-Amino-4*H*-3,1-benzothiazine; *N*-Et, *in* A-70092

$C_{10}H_{12}N_4$
2,4,6,7-Tetramethylpteridine, T-70142

$C_{10}H_{12}N_4O_2$
▷ Tris(2-cyanoethyl)nitromethane, *in* C-80025

$C_{10}H_{12}N_4O_3$
Leucettidine, L-70029
2,4,7(1*H*,3*H*,8*H*)-Pteridinetrione; 1,3,6,8-Tetra-Me, *in* P-70135

$C_{10}H_{12}N_4O_4$
2′-Deoxyinosine, D-70023
2′-Deoxyinosine, D-80029
3′-Deoxyinosine, D-70024

$C_{10}H_{12}N_4O_4S$
▷ 6-Mercaptopurine; 9-β-D-Ribofuranosyl, *in* D-60270
▷ 6-Thioinosine, T-70180

$C_{10}H_{12}N_4O_6$
Tetrahydro-1,2,4,5-tetrazine-3,6-dione; 1,2,4,5-Tetra-Ac, *in* T-70097

$C_{10}H_{12}N_6$
6,6′-Dihydroxy-2,2′-bipyridine; Dihydrazone, *in* D-80299

$C_{10}H_{12}O$
1-Ethoxy-1-phenylethylene, *in* P-60092
▷ 1-Methoxy-4-(1-propenyl)benzene, *in* P-80179
1-Phenyl-3-buten-1-ol, P-70061
4-Phenyl-3-buten-1-ol, P-80097
1,2,4,5-Tetrahydro-3-benzoxepin, T-70043
1,3,4,5-Tetrahydro-2-benzoxepin, T-70044
2,3,4,5-Tetrahydro-1-benzoxepin, T-70045
3,4,5,6-Tetrahydro-1(2*H*)-naphthalenone, T-80075

$C_{10}H_{12}OS$
Benzeneethanethioic acid; *O*-Et ester, *in* B-70017
Benzeneethanethioic acid; *S*-Et ester, *in* B-70017
Tetrahydro-3-(phenythio)furan, *in* T-80063

$C_{10}H_{12}O_2$
3,4-Dihydro-2*H*-1-benzopyran-7-ol; Me ether, *in* D-60202
3,4-Dihydro-6-methoxy-2*H*-1-benzopyran, *in* D-70175
3,4-Dihydro-8-methoxy-2*H*-1-benzopyran, *in* D-60203
Dispiro[cyclopropane-1,5′-[3,8]dioxatricyclo[5.1.0.0^{2,4}]octane-6′,1″-cyclopropane], D-60500
1-Ethenyl-2,4-dimethoxybenzene, *in* V-70010
Fusalanipyrone, F-80099
1,3,4,5,7,8-Hexahydro-2,6-naphthalenedione, H-70063
1-(4-Methoxyphenyl)-2-propanone, *in* H-80241
2-(2-Methylphenyl)propanoic acid, M-60113
2-(4-Methylphenyl)propanoic acid, M-60114
3,4,5-Trimethylbenzoic acid, T-60355

$C_{10}H_{12}O_2S$
2-Mercapto-3-phenylpropanoic acid; Me ester, *in* M-60026
3-(Phenylthio)butanoic acid, *in* M-70023

$C_{10}H_{12}O_3$
Adriadysiolide, A-70069
Anisyl acetate, *in* H-80114
2-*O*-Benzylglyceraldehyde, B-80058
2,5-Dimethoxybenzeneacetaldehyde, *in* D-60370
3,4-Dimethoxybenzeneacetaldehyde, *in* D-60371
2-Hydroxy-4-methylbenzoic acid; Et ester, *in* H-70163
4-Hydroxy-2-methylbenzoic acid; Et ester, *in* H-70164

$C_{10}H_{12}O_3S$
3-(Phenylsulfinyl)butanoic acid, *in* M-70023

$C_{10}H_{12}O_4$
1,4-Benzoquinone; Bis(ethylene ketal), *in* B-70044
4,5-Dimethoxy-2-methylbenzoic acid, *in* D-80339
6-Ethyl-2,4-dihydroxy-3-methylbenzoic acid, E-70041
Hallerone, H-60005
2′-Hydroxy-4′,6′-dimethoxyacetophenone, *in* T-70248
▷ 1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone, *in* T-60315
(3-Hydroxyphenoxy)acetic acid; Et ester, *in* H-70204

$C_{10}H_{12}O_5$
2,5-Bis(hydroxymethyl)furan; Di-Ac, *in* B-60160
3,4-Bis(hydroxymethyl)furan; Di-Ac, *in* B-60161
Gelsemide, G-60010
3-Hydroxy-4,6-dimethoxy-2-methylbenzoic acid, *in* T-80324
2,3,5-Trimethoxybenzoic acid, *in* T-70250

$C_{10}H_{12}S_8$
Tetramercaptotetrathiafulvalene; Tetrakis(*S*-Me), *in* T-70130

$C_{10}H_{13}BrCl_2$
2-Bromo-4-chloro-1-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane, B-80185

$C_{10}H_{13}I$
1-*tert*-Butyl-2-iodobenzene, B-60346
1-*tert*-Butyl-3-iodobenzene, B-60347
1-*tert*-Butyl-4-iodobenzene, B-60348

$C_{10}H_{13}N$
Azetidine; *N*-Benzyl, *in* A-70283
2,3,4,5-Tetrahydro-1*H*-1-benzazepine, T-70036

$C_{10}H_{13}NO$
2-(4-Methylphenyl)propanoic acid; Amide, *in* M-60114
1,2,3,4-Tetrahydro-5-hydroxyisoquinoline; Me ether; BHCl, *in* T-80065
7,8,9,10-Tetrahydropyrido[1,2-*a*]azepin-4(6*H*)-one, T-60085
Weberidine, *in* T-80066

$C_{10}H_{13}NO_2$
2-Amino-2-methyl-3-phenylpropanoic acid, A-60225
3-Amino-2,4,6-trimethylbenzoic acid, A-60266
5-Amino-2,3,4-trimethylbenzoic acid, A-60267

$C_{10}H_{13}NO_3$
4-Amino-1,2-benzenediol; Di-Me ether, *N*-Ac, *in* A-70090
2-Amino-2-methyl-3-(4-hydroxyphenyl)propanoic acid, A-60220

$C_{10}H_{13}NO_4$
2-Amino-3-hydroxy-4-(4-hydroxyphenyl)butanoic acid, A-60185
1*H*-Pyrrole-3,4-dicarboxylic acid; Di-Et ester, *in* P-70183
2′,4′,6′-Trihydroxyacetophenone; 2′,4′-Di-Me ether, oxime, *in* T-70248

$C_{10}H_{13}NO_5$
3-Hydroxy-1*H*-pyrrole-2,4-dicarboxylic acid; Di-Et ester, *in* H-80251

$C_{10}H_{13}N_5O_3$
2-Amino-6-(1,2-dihydroxypropyl)-3-methylpterin-4-one, A-60146
2-Amino-6-(1,2-dihydroxypropyl)-3-methylpterin-4-one, *in* B-70121

$C_{10}H_{13}N_5O_4$
3′-Azido-3′-deoxythymidine, A-80197
9-β-D-Ribofuranosyl-9*H*-purin-2-amine, *in* A-60243

$C_{10}H_{13}N_5O_5$
6-Amino-1,3-dihydro-2*H*-purin-2-one; 9-(β-D-Arabinofuranosyl), *in* A-60144
8-Amino-9-β-D-ribofuranosyl-6*H*-purin-6-one, A-70198

$C_{10}H_{13}N_5O_5S$
8-Mercaptoguanosine, M-70029

$C_{10}H_{13}N_5O_6$
7,8-Dihydro-8-oxoguanosine, D-70238

$C_{10}H_{14}$
5,5′-Bibicyclo[2.1.0]pentane, B-70092
2,3-Dimethylenebicyclo[2.2.2]octane, D-70408
1-Ethynylbicyclo[2.2.2]octane, E-70049
1,2,3,5,8,8*a*-Hexahydronaphthalene, H-60053
1,2,3,7,8,8*a*-Hexahydronaphthalene, H-60054
2-Methyl-6-methylene-1,3,7-octatriene, M-60089
Tricyclo[4.3.1.0^{3,8}]dec-4-ene, T-80236
Tricyclo[5.2.1.0^{2,6}]dec-2(6)-ene, T-60260

$C_{10}H_{14}BrCl_3$
Coccinene/, *in* M-80035
Mertensene, M-80035
Telfairine, T-80005

$C_{10}H_{14}BrNO_2$
2-Bromo-2-nitroadamantane, B-80234

$C_{10}H_{14}Br_2$
1,3-Dibromoadamantane, D-70084

$C_{10}H_{14}Br_2Cl_2$
4,8-Dibromo-3,7-dichloro-3,7-dimethyl-1,5-octadiene, D-80086

$C_{10}H_{14}Br_3Cl_3$
1,5,7-Tribromo-2,6,8-trichloro-2,6-dimethyl-3-octene, T-80218

$C_{10}H_{14}ClNO_2$
2-Chloro-2-nitroadamantane, C-80082

$C_{10}H_{14}Cl_4$
Gelidene, G-80006
1,2,4-Trichloro-5-(2-chloroethenyl)-1,5-dimethylcyclohexane, T-80223

$C_{10}H_{14}IN$
4-Iodo-3,5-dimethylaniline; *N*,*N*-Di-Me, *in* I-70031

$C_{10}H_{14}N_2O_2$
2,4-Dihydroxyphenylacetaldehyde; Dimethylhydrazone, *in* D-60369
Octahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60016

$C_{10}H_{14}N_2O_3$
Octahydro-2-hydroxy-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60017

$C_{10}H_{14}N_2O_4$
2,2-Dinitroadamantane, D-50699
2,4-Dinitroadamantane, D-80489
2,6-Dinitroadamantane, D-80490
1-[3-Hydroxy-4-(hydroxymethyl)cyclopentyl]-2,4(1*H*,3*H*)-pyrimidinedione, H-70140
Isoporphobilinogen, I-60114
Octahydro-5*a*,10*a*-dihydroxy-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60014
Octahydro-2,7-dihydroxy-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, O-60013
1*H*-Pyrazole-4,5-dicarboxylic acid; 1-Me, Di-Et ester, *in* P-80199

$C_{10}H_{14}N_2S_2$
Octahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dithione, O-70014

$C_{10}H_{14}N_6O_3$
3′-Amino-3′-deoxyadenosine, A-70128

$C_{10}H_{14}N_6O_5$
8-Aminoguanosine, A-70150

$C_{10}H_{14}O$
1-Acetyl-4-isopropenylcyclopentene, A-80025
1-Acetyl-4-isopropylidenecyclopentene, A-80026
3-Caren-5-one, C-60019
2,7-Cyclodecadien-1-one, C-60185
3,7-Cyclodecadien-1-one, C-60186
2-Cyclopentylidenecyclopentanone, C-60227
3,3-Dimethylbicyclo[2.2.2]oct-5-en-2-one, D-60412
3,4,4*a*,5,8,8*a*-Hexahydro-1(2*H*)-naphthalenone, H-80061
4*a*,5,6,7,8,8*a*-Hexahydro-2(1*H*)-naphthalenone, H-80062
6-Isopropenyl-3-methyl-2-cyclohexen-1-one, I-70088
▷ 4-Isopropylbenzyl alcohol, I-80078
5-Methoxy-1,2,3-trimethylbenzene, *in* T-60371
7-Methylenebicyclo[3.3.1]nonan-3-one, M-70062
Myrtenal, *in* M-80205
Tricyclo[4.4.0.0^{3,8}]decan-4-one, T-80235
2,3,5-Trimethylbenzyl alcohol, T-80349
3,4,5-Trimethylbenzyl alcohol, T-80350

$C_{10}H_{14}O_2$
2-Benzyloxy-1-propanol, *in* P-70118
1-Cycloheptenecarboxylic acid; Et ester, *in* C-80178
4,4-Dimethylbicyclo[3.2.1]octane-2,3-dione, D-60410
3-Ethynyl-3-methyl-4-pentenoic acid; Et ester, *in* E-60059
▷ 1-(3-Furanyl)-4-methyl-1-pentanone, F-60087
2-Hydroxy-1(10)-pinen-5-one, H-80247
Isoneonepetalactone, *in* N-70027
2-Isopropyl-5-methyl-1,3-benzenediol, I-60122
2-Isopropyl-6-methyl-1,4-benzenediol, I-60123
3-Isopropyl-6-methyl-1,2-benzenediol, I-60124
5-Isopropyl-2-methyl-1,3-benzenediol, I-60125
5-Isopropyl-3-methyl-1,2-benzenediol, I-60126
5-Isopropyl-4-methyl-1,3-benzenediol, I-60127
Neonepetalactone, N-70027
Nepetalactone, N-60020
4-Oxatricyclo[4.3.1.1^{3,8}]undecan-5-one, O-60055
2-Pinen-10-oic acid, *in* M-80205
3,3,6,6-Tetramethyl-4-cyclohexene-1,2-dione, T-60134
5,5,6,6-Tetramethyl-2-cyclohexene-1,4-dione, T-60135

$C_{10}H_{14}O_3$
2,5-Dihydroxy-4-isopropylbenzyl alcohol, D-70309
2-(Dimethoxymethyl)benzenemethanol, *in* H-60171
α-(Dimethoxymethyl)benzenemethanol, *in* H-60210
Peperinic acid, P-80063

$C_{10}H_{14}O_4$
2-Cyclohexene-1,4-diol; Di-Ac, *in* C-80181
4-Cyclohexene-1,2-diol; Di-Ac, *in* C-80182
1,2,3,4-Tetramethoxybenzene, *in* B-60014
3,4,5-Trimethoxybenzyl alcohol, *in* H-80196

$C_{10}H_{14}O_5$
Hexahydro-3,7*a*-dihydroxy-3*a*,7-dimethyl-1,4-isobenzofurandione, H-70055
3-(5-Hydroxymethyl-5-methyl-2-oxo-5*H*-furan-3-yl)-2-methylpropanoic acid, H-80208

$C_{10}H_{14}S_2$
1,4-Dimethyl-2,5-bis(methylthio)benzene, *in* D-60406

$C_{10}H_{15}BrCl_2O$
Aplysiapyranoid *C*, A-70245
Aplysiapyranoid *D*, *in* A-70245

$C_{10}H_{15}Br_2Cl$
7,8-Dibromo-6-(chloromethylene)-2-methyl-2-octene, D-70088

$C_{10}H_{15}Br_2ClO$
Aplysiapyranoid *A*, A-70244
Aplysiapyranoid *B*, *in* A-70244

$C_{10}H_{15}Cl$
1-Chloroadamantane, C-60039
2-Chloroadamantane, C-60040

$C_{10}H_{15}ClO_5$
Jioglutin A, J-80010
Jioglutin B, *in* J-80010

$C_{10}H_{15}Cl_3$
1,8-Dichloro-6-chloromethyl-2-methyl-2,6-octadiene, D-70116
3,8-Dichloro-6-chloromethyl-2-methyl-1,6-octadiene, D-70117

$C_{10}H_{15}NO$
2-Cyclopentylidenecyclopentanone; Oxime, *in* C-60227
3-Ethynyl-3-methyl-4-pentenoic acid; *N,N*-Dimethylamide, *in* E-60059
4*a*,5,6,7,8,8*a*-Hexahydro-2(1*H*)-naphthalenone; Oxime, *in* H-80062

$C_{10}H_{15}NO_2$
3,4,4*a*,5,8,8*a*-Hexahydro-1(2*H*)-naphthalenone; Oxime, *in* H-80061
1-Nitroadamantane, N-80033
2-Nitroadamantane, N-80034

$C_{10}H_{15}NO_4$
α-Allokainic acid, *in* K-60003
▷ Kainic acid, K-60003

$C_{10}H_{15}NO_7$
2-Amino-1,1,2-ethanetricarboxylic acid; *N*-Ac, Tri-Me ester, *in* A-80072

$C_{10}H_{15}NO_8$
4-(2-Carboxyethyl)-4-nitroheptanedioic acid, C-80025

$C_{10}H_{15}N_2O_8P$
Thymidine 5′-phosphate, T-80196

$C_{10}H_{15}N_3$
2-Azidoadamantane, A-60337

$C_{10}H_{15}N_3O_2$
1*H*-Pyrrole-3,4-dicarboxylic acid; Dimethylamide, *in* P-70183

$C_{10}H_{15}N_3O_4$
Carbodine, C-70018

$C_{10}H_{15}N_3O_5$
Homocytidine, *in* A-70130

$C_{10}H_{16}$
Bicyclo[6.2.0]dec-9-ene, B-80074
1-*tert*-Butyl-1,3-cyclohexadiene, B-70296
4-Decen-1-yne, D-70020
1,2-Diethylidenecyclohexane, D-70154
4-Isopropenyl-1-methylcyclohexene, I-70087
3-Isopropylidene-6-methylcyclohexene, I-80081
3,3,6,6-Tetramethylcyclohexyne, T-70132
3-Thujene, T-80194
4(10)-Thujene, T-80195

$C_{10}H_{16}Cl_2$
1-Chloro-3-(chloromethyl)-7-methyl-2,6-octadiene, C-70060

$C_{10}H_{16}Cl_2O_2$
2,2-Dichloro-7-octenoic acid; Et ester, *in* D-80123

$C_{10}H_{16}N_2S_2$
4,6-Diamino-1,3-benzenedithiol; Di-*S*-Et, *in* D-70037

$C_{10}H_{16}N_2S_4$
2,3,5,6-Tetrakis(methylthio)-1,4-benzenediamine, *in* D-60031

$C_{10}H_{16}N_4$
2,3,5,6,8,9-Hexahydro-1*H*-diimidazo[1,2-*d*:2′,1′-*g*][1,4]diazepine; *N*-Me, *in* H-80058

$C_{10}H_{16}O$
1-Acetylcyclooctene, A-60027
3-*tert*-Butyl-2-cyclohexen-1-one, B-70297
3,3-Dimethylbicyclo[2.2.2]octan-2-one, D-60411
2-Isopropyl-5-methyl-4-cyclohexen-1-one, I-60128
2-Methyl-6-methylene-2,7-octadien-4-ol, M-70093
Myrtenol, M-80205
2-(2-Propenyl)cycloheptanone, P-80176
2,2,5,5-Tetramethyl-3-cyclohexen-1-one, T-60136

$C_{10}H_{16}O_2$
Bicyclo[3.2.1]octane-1-carboxylic acid; Me ester, *in* B-70112
1-Cyclooctene-1-acetic acid, C-70241
4-Cyclooctene-1-acetic acid, C-70242
2,5,8-Decatriene-1,10-diol, D-80015
Eldanolide, E-70004
2,3-Epoxy-5,7-octadien-4-ol, E-80042
2-Hydroperoxy-2-methyl-6-methylene-3,7-octadiene, H-60097
3-Hydroperoxy-2-methyl-6-methylene-1,7-octadiene, H-60098
Iridodial, I-60084
Lineatin, L-60027
3-Myodeserten-1-ol, M-80203
Piperitone oxide, P-80153
Spiro[bicyclo[3.2.1]octane-8,2′-[1,3]dioxolane], *in* B-60094

$C_{10}H_{16}O_3$
1,7-Dihydroxy-3,7-dimethyl-2,5-octadien-4-one, D-60318
3-Hydroxy-4-(hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptan-2-one, *in* H-70173
9-Oxo-2-decenoic acid, O-70089
Secothujene, S-70027

$C_{10}H_{16}O_4$
Gelsemiol, G-60011
3-Hexene-2,5-diol; Di-Ac, *in* H-80083
7-Hydroxy-1-hydroxy-3,7-dimethyl-2*E*,5*E*-octadien-4-one, *in* D-60318
2,2,5,5-Tetramethyl-3-hexenedioic acid, T-60141

$C_{10}H_{16}O_6$
Jioglutin C, J-80011

$C_{10}H_{16}S$
2-Adamantanethiol, A-80038

$C_{10}H_{16}S_2$
1,3-Bis(allylthio)cyclobutane, *in* C-60184

$C_{10}H_{17}N$
4-Azatricyclo[4.3.1.1^{3,8}]undecane, A-60333
Decahydro-1*H*-dicyclopenta[*b*,*d*]pyrrole, D-80010

$C_{10}H_{17}NO_3$
2-Nitrocyclodecanone, N-70046

$C_{10}H_{18}$
1-*tert*-Butylcyclohexene, B-60341
3-*tert*-Butylcyclohexene, B-60342
4-*tert*-Butylcyclohexene, B-60343

$C_{10}H_{18}BrN$
1-Azoniatricyclo[3.3.3.0]undecane; Bromide, *in* A-80206

$C_{10}H_{18}Br_2$
2,2-Dibromo-1,1,3,3-tetramethylcyclohexane, D-80101

$C_{10}H_{18}ClN$
1-Azoniatricyclo[3.3.3.0]undecane; Chloride, *in* A-80206

$C_{10}H_{18}N^{\oplus}$
1-Azoniatricyclo[3.3.3.0]undecane, A-80206

$C_{10}H_{18}N_2O_2$
1,1-Di-4-morpholinylethene, D-70447

$C_{10}H_{18}N_2O_4$
2*H*-1,5,2,4-Dioxadiazine-3,6(4*H*)dione; 2,4-Di-*tert*-butyl, *in* D-60466

$C_{10}H_{18}N_2O_6S_2$
γ-Glutamylmarasmine, G-60026

$C_{10}H_{18}N_4O_4$
1,2-Dihydrazinoethane; N^{α},$N^{\alpha'}$,N^{β},$N^{\beta'}$-Tetra-Ac, *in* D-60192

$C_{10}H_{18}O$
1-*tert*-Butoxy-1-hexyne, B-80282
3-Decenal, D-70016
3,7-Dimethyl-6-octenal, D-60430
4,6-Dimethyl-4-octen-3-one, D-70424
Hexamethylcyclobutanone, H-60069
2-Isopropylcycloheptanone, I-70090
4-Isopropylcycloheptanone, I-70091
1-Methoxy-2-nonyne, *in* N-80074
2-Methyl-6-methylene-7-octen-4-ol, *in* M-70093
Tetrahydro-2,2-dimethyl-5-(1-methyl-1-propenyl)furan, T-80061
2,2,6,6-Tetramethylcyclohexanone, T-60133
2,2,6-Trimethyl-5-hepten-3-one, T-60365

$C_{10}H_{18}OS$
Di-*tert*-butylthioketene; *S*-Oxide, *in* D-60114

$C_{10}H_{18}O_2$
4-Decenoic acid, D-80017
3,6-Diethoxycyclohexene, *in* C-80181
3,4-Diethoxy-1,5-hexadiene, *in* H-70036
Dihydro-4-methyl-5-pentyl-2(3*H*)-furanone, D-80227
4,4-Dimethyl-6-heptenoic acid; Me ester, *in* D-80450
2,6-Dimethyl-2,7-octadiene-1,6-diol, D-80456
2,6-Dimethyl-3,7-octadiene-2,6-diol, D-70422
3,7-Dimethyl-2,5-octadiene-1,7-diol, D-80457
▷ 5-Hexyldihydro-2(3*H*)-furanone, H-60078
2-Hydroxy-1,4-cineole, H-80139
6-Hydroxydecanoic acid; Lactone, *in* H-80147
4-Isopropenyl-1-methyl-1,2-cyclohexanediol, I-70086
4-Isopropyl-1-methyl-4-cyclohexene-1,2-diol, I-70094
4-Isopropyl-1-methyl-3-cyclohexenene-1,2-diol, I-70093
p-Menth-4-ene-1,2-diol, M-80014
p-Menth-3-ene-1,2-diol, M-80015
p-Menth-7-ene-1,2-diol, M-80016
10-Methyl-2-oxecanone, *in* H-80149
2-Octen-1-ol; Ac, *in* O-60029
2,2,5,5-Tetramethyl-3,4-hexanedione, T-80146
1,7,7-Trimethylbicyclo[2.2.1]heptane-2,5-diol, T-70280

$C_{10}H_{18}O_3$
1,7-Bis(hydroxymethyl)-7-methylbicyclo[2.2.1]heptan-2-ol, B-70146
2-Hydroxy-4-*tert*-butylcyclopentanecarboxylic acid, H-70113
1-(Hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptane-2,3-diol, H-70173
9-Hydroxy-5-nonenoic acid; Me ester, *in* H-70194
6-Methyl-5-oxoheptanoic acid; Et ester, *in* M-80130
10-Oxodecanoic acid, O-60063

$C_{10}H_{18}O_4$
3-Methyl-4-oxo-2-butenoic acid; Me ester, di-Et acetal, *in* M-70103
Nonactinic acid, N-70069

$C_{10}H_{18}O_5$
Methyl hydrogen 2-(*tert*-butoxymethyl)-2-methylmalonate, M-70088

$C_{10}H_{18}S$
Di-*tert*-butylthioketene, D-60114

$C_{10}H_{19}Br$
5-Bromo-5-decene, B-60225

$C_{10}H_{19}NO$
1-Oxa-2-azaspiro[2,5]octane; *N*-*tert*-Butyl, *in* O-70052
2,2,6,6-Tetramethylcyclohexanone; Oxime, *in* T-60133

$C_{10}H_{19}NO_2$
3-Amino-2-hexenoic acid; *tert*-Butyl ester, *in* A-60170

$C_{10}H_{19}NO_3$
2-Amino-1-hydroxy-1-cyclobutaneacetic acid; *tert*-Butyl ester, *in* A-60184
2-Amino-3-hydroxy-4-methyl-6-octenoic acid; *N*-Me, *in* A-60189
10-Oxodecanoic acid; Oxime, *in* O-60063

$C_{10}H_{19}N_3$
1*H*,4*H*,7*H*,9*bH*-2,3,5,6,8,9-Hexahydro-3*a*,6*a*,9*a*-triazaphenalene, H-70078

$C_{10}H_{20}$
5-Decene, D-70017
Methylcyclononane, M-60058

$C_{10}H_{20}N_2$
1,5-Diazabicyclo[5.2.2]undecane; *N*-Me, *in* D-60055

$C_{10}H_{20}N_2O$
N,*N*-Diethyl-3-piperidinecarboxamide, *in* P-70102

$C_{10}H_{20}N_2S_2$
▷ 1,1′-Dithiobispiperidine, D-70523

$C_{10}H_{20}N_4$
▷ 6*H*,13*H*-Octahydrodipyridazino[1,2-*a*:1′,2′-*d*][1,2,4,5]tetrazine, O-70013

$C_{10}H_{20}O$
5-Decanone, D-60014
2-Decen-4-ol, D-60016
5-Decen-1-ol, D-70019
6-Decen-1-ol, D-80018
2,2,3,3,4,4-Hexamethylcyclobutanol, H-60068
7-Methyl-3-methylene-1-octanol, M-80118

$C_{10}H_{20}O_2$
2,5-Diethoxy-3-hexene, *in* H-80083
1-Isopropyl-4-methyl-1,4-cyclohexanediol, I-80082

$C_{10}H_{20}O_3$
6-Hydroxydecanoic acid, H-80147
7-Hydroxydecanoic acid, H-80148
9-Hydroxydecanoic acid, H-80149

$C_{10}H_{20}O_4$
3,4-Dihydroxybutanoic acid; O^4-*tert*-Butyl, Et ester, *in* D-60313
Tetraethoxyethene, T-80047

$C_{10}H_{20}O_5$
Di-*tert*-butyl dicarbonate, *in* D-70111

$C_{10}H_{21}N$
Octahydroazocine; 1-Isopropyl, *in* O-70010

$C_{10}H_{22}N_2$
Hexahydropyrimidine; 1,3-Diisopropyl, *in* H-60056

$C_{10}H_{22}N_2O_3$
1,4,10-Trioxa-7,13-diazacyclopentadecane, T-60376

$C_{10}H_{22}N_2O_5$
6,10-Diamino-2,3,5-trihydroxydecanoic acid, D-70046

$C_{10}H_{22}N_4O_2S_2$
Alethine, A-60073

$C_{10}H_{22}O_2$
5,6-Decanediol, D-60013

$C_{10}H_{22}O_9$
Lacticolorin, *in* D-80284

$C_{10}H_{23}NO_3$
4-Amino-4-(3-hydroxypropyl)-1,7-heptanediol, A-80085

$C_{10}H_{23}N_3$
1,5,9-Triazacyclotridecane, T-60233

$C_{10}H_{25}N_5$
1,4,7,10,13-Pentaazacyclopentadecane, P-60025

$C_{11}H_5Cl_{11}$
Chloropentakis(dichloromethyl)benzene, C-70136

$C_{11}H_5NO_3$
2,3-Quinolinedicarboxylic acid; Anhydride, *in* Q-80002

$C_{11}H_6N_2O$
3,6-Diazafluorenone, D-70053

$C_{11}H_6N_2OS$
10*H*-[1]Benzothiopyrano[2,3-*d*]pyridazin-10-one, B-80045

$C_{11}H_6N_2O_2$
10*H*-[1]Benzopyrano[2,3-*b*]pyrazin-10-one, B-80035
10*H*-[1]Benzopyrano[2,3-*d*]pyridazin-10-one, B-80037
2,3-Quinolinedicarboxylic acid; Imide, *in* Q-80002

$C_{11}H_6N_4$
9-Diazo-9*H*-cyclopenta[1,2-*b*:4,3-*b*′]dipyridine, D-60059

$C_{11}H_6N_6$
Pyrimido[4,5-*i*]imidazo[4,5-*g*]cinnoline, P-60244

$C_{11}H_6O$
1-Phenyl-1,4-pentadiyn-3-one, P-70087
1-Phenyl-2,4-pentadiyn-1-one, P-80114

$C_{11}H_6OS$
Naphtho[2,1-*b*]thiet-1-one, N-70013

$C_{11}H_7BrO$
1-Bromo-2-naphthalenecarboxaldehyde, B-60302

$C_{11}H_7BrO_3$
3-Bromo-5-hydroxy-2-methyl-1,4-naphthoquinone, B-60266
2-Bromo-6-methoxy-1,4-naphthaquinone, *in* B-60270
2-Bromo-3-methoxy-1,4-naphthoquinone, *in* B-60268
2-Bromo-5-methoxy-1,4-naphthoquinone, *in* B-60269
2-Bromo-7-methoxy-1,4-naphthoquinone, *in* B-60271
2-Bromo-8-methoxy-1,4-naphthoquinone, *in* B-60272

$C_{11}H_7ClN_2$
2-Chloro-1*H*-perimidine, C-80092

$C_{11}H_7ClO_3$
3-Chloro-5-hydroxy-2-methyl-1,4-naphthoquinone, C-60098
2-Oxo-2*H*-benzopyran-4-acetic acid; Chloride, *in* O-60057

$C_{11}H_7NO$
Benz[*cd*]indol-2-(1*H*)-one, B-70027
3*H*-Pyrrolo[1,2-*a*]indol-3-one, P-80227
9*H*-Pyrrolo[1,2-*a*]indol-9-one, P-60247

$C_{11}H_7NOSe$
[1,4]Benzoxaselenino[3,2-*b*]pyridine, B-60054

$C_{11}H_7NO_2$
[1,4]Benzodioxino[2,3-*b*]pyridine, B-80021
4-(Cyanomethyl)coumarin, *in* O-60057
4-Oxo-4*H*-1-benzopyran-3-acetic acid; Nitrile, *in* O-60059
Pyrano[3,4-*b*]indol-3(9*H*)-one, P-80196

$C_{11}H_7NO_3$
3-Nitro-2-naphthaldehyde, N-70054

$C_{11}H_7NO_4$
2,3-Quinolinedicarboxylic acid, Q-80002

$C_{11}H_7NS$
Azuleno[1,2-*d*]thiazole, A-60356
Azuleno[2,1-*d*]thiazole, A-60357
Naphtho[1,8-*de*]-1,3-thiazine, N-80009
2-(Phenylethynyl)thiazole, P-60099
4-(Phenylethynyl)thiazole, P-60100

$C_{11}H_7N_3O$
Pyridazino[4,5-*b*]quinolin-10(5*H*)-one, P-80207

$C_{11}H_7N_3O_2$
Pyrimido[4,5-*b*]quinoline-2,4(3*H*,10*H*)-dione, P-60245

$C_{11}H_8$
5-Phenyl-1,3-pentadiyne, P-80113

$C_{11}H_8BrN$
2-Bromo-4-phenylpyridine, B-80245
2-Bromo-5-phenylpyridine, B-80246
2-Bromo-6-phenylpyridine, B-80247

3-Bromo-2-phenylpyridine, B-80248
3-Bromo-4-phenylpyridine, B-80249
4-Bromo-2-phenylpyridine, B-80250
5-Bromo-2-phenylpyridine, B-80251

$C_{11}H_8Br_2$
▷ 1-Bromo-2-(bromomethyl)naphthalene, B-60212
1-Bromo-4-(bromomethyl)naphthalene, B-60213
1-Bromo-5-(bromomethyl)naphthalene, B-60214
1-Bromo-7-(bromomethyl)naphthalene, B-60215
1-Bromo-8-(bromomethyl)naphthalene, B-60216
2-Bromo-3-(bromomethyl)naphthalene, B-60217
2-Bromo-6-(bromomethyl)naphthalene, B-60218
3-Bromo-1-(bromomethyl)naphthalene, B-60219
6-Bromo-1-(bromomethyl)naphthalene, B-60220
7-Bromo-1-(bromomethyl)naphthalene, B-60221
1,2-Dibromo-1,4-dihydro-1,4-methanonaphthalene, D-60095
1,3-Dibromo-1,4-dihydro-1,4-methanonaphthalene, D-60096

$C_{11}H_8ClNO_2$
Silital, *in* C-70075

$C_{11}H_8N_2$
1*H*-Benzo[*de*][1,6]naphthyridine, B-70037
7-Diazo-7*H*-benzocycloheptene, D-80064

$C_{11}H_8N_2O$
Di-2-pyridyl ketone, D-70502
Di-3-pyridyl ketone, D-70503
Di-4-pyridyl ketone, D-70504
1*H*-Indole-3-carboxylic acid; Nitrile, *N*-Ac, *in* I-80012
1*H*-Perimidin-2(3*H*)-one, P-70043
2-Pyridyl 3-pyridyl ketone, P-70179
2-Pyridyl 4-pyridyl ketone, P-70180
3-Pyridyl 4-pyridyl ketone, P-70181

$C_{11}H_8N_2O_2$
5-Benzoyl-2(1*H*)-pyrimidinone, B-60066

$C_{11}H_8N_2O_2S$
1,1′-Carbonothioylbis-2(1*H*)pyridinone, C-60014

$C_{11}H_8N_2O_3S$
1*H*-Perimidine-2-sulfonic acid, P-80067

$C_{11}H_8N_2S$
Dipyrido[1,2-*a*: 1′,2′-*c*]imidazolium-11-thiolate, D-80516
1*H*-Perimidine-2(3*H*)-thione, P-10051

$C_{11}H_8N_4$
1*H*-Pyrazolo[3,4-*d*]pyrimidine; 1-Ph, *in* P-70156

$C_{11}H_8N_4O$
1*H*-Pyrazolo[3,4-*d*]pyrimidine; 1-Ph, 5-oxide, *in* P-70156

$C_{11}H_8OS_2$
5-(2-Thienylethynyl)-2-thiophenemethanol, T-80180

$C_{11}H_8O_2$
Homoazulene-1,5-quinone, H-60085
Homoazulene-1,7-quinone, H-60086
Homoazulene-4,7-quinone, H-60087
6-Hydroxy-1-naphthaldehyde, H-70184
6-Hydroxy-2-naphthaldehyde, H-70185
7-Hydroxy-2-naphthaldehyde, H-70186

$C_{11}H_8O_3$
2-Acetyl-4*H*-1-benzopyran-4-one, A-80016
3-Acetyl-4*H*-1-benzopyran-4-one, A-80017
5-Hydroxy-7-methyl-1,2-naphthoquinone, H-60189
8-Hydroxy-3-methyl-1,2-naphthoquinone, H-60190
4-Methoxy-1,2-naphthoquinone, *in* H-60194
Pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane-4,8,11-trione, P-70023
Pentacyclo[6.3.0.0^{2,6}.0^{5,9}]undecane-4,7,11-trione, P-60031
2-Phenyl-3-furancarboxylic acid, P-70076
4-Phenyl-2-furancarboxylic acid, P-70077
5-Phenyl-2-furancarboxylic acid, P-70078

$C_{11}H_8O_4$
3,5-Dihydroxy-2-methyl-1,4-naphthoquinone, D-60350
5,6-Dihydroxy-2-methyl-1,4-naphthoquinone, D-60351
3-(6-Hydroxy-5-benzofuranyl)-2-propenoic acid, H-80113
2-Hydroxy-8-methoxy-1,4-naphthoquinone, *in* D-60355
4-Methyl-6,7-methylenedioxy-2*H*-1-benzopyran-2-one, M-70092
1-Oxo-1*H*-2-benzopyran-3-acetic acid, O-60058
2-Oxo-2*H*-benzopyran-4-acetic acid, O-60057
4-Oxo-4*H*-1-benzopyran-3-acetic acid, O-60059

$C_{11}H_8O_5$
4-Hydroxy-5-benzofurancarboxylic acid; Ac, *in* H-60103
2-Hydroxy-5-methoxy-1,4-naphthoquinone, *in* D-60354

$C_{11}H_8O_8$
2,3,5,6,8-Pentahydroxy-7-methoxy-1,4-naphthoquinone, *in* H-60065

$C_{11}H_9BF_4N_4$
3-Phenyltetrazolo[1,5-*a*]pyridinium; Tetrafluoroborate, *in* P-60134

$C_{11}H_9Br$
1-Bromo-1,4-dihydro-1,4-methanonaphthalene, B-60231
2-Bromo-1,4-dihydro-1,4-methanonaphthalene, B-60232
9-Bromo-1,4-dihydro-1,4-methanonaphthalene, B-60233

$C_{11}H_9BrN_2$
Dipyrido[1,2-*a*:1′,2′-*c*]imidazol-10-ium(1+); Bromide, *in* D-70501

$C_{11}H_9BrN_4$
3-Phenyltetrazolo[1,5-*a*]pyridinium; Bromide, *in* P-60134

$C_{11}H_9BrO$
1-Bromo-3,4-dihydro-2-naphthalenecarboxaldehyde, B-80197
2-Bromo-3,4-dihydro-1-naphthalenecarboxaldehyde, B-80198

$C_{11}H_9ClN_2O_4$
Dipyrido[1,2-*a*:1′,2′-*c*]imidazol-10-ium(1+); Perchlorate, *in* D-70501

$C_{11}H_9I$
2-(Iodomethyl)naphthalene, I-80035

$C_{11}H_9IN_2$
Dipyrido[1,2-*a*:1′,2′-*c*]imidazol-10-ium(1+); Iodide, *in* D-70501

$C_{11}H_9N$
2-Ethynylindole; 1-Me, *in* E-60057
4-Vinylquinoline, V-70014

$C_{11}H_9NO$
1-Acetylisoquinoline, A-60039
3-Acetylisoquinoline, A-60040
4-Acetylisoquinoline, A-60041
5-Acetylisoquinoline, A-60042
2-Acetylquinoline, A-60049
3-Acetylquinoline, A-60050
4-Acetylquinoline, A-60051
5-Acetylquinoline, A-60052
6-Acetylquinoline, A-60053
7-Acetylquinoline, A-60054
8-Acetylquinoline, A-60055
2-Phenyl-1,3-oxazepine, P-60123
5-Phenyl-1,4-oxazepine, P-60124

$C_{11}H_9NO_2$
4-Acetylquinoline; 1-Oxide, *in* A-60051
2-Amino-3-methyl-1,4-naphthoquinone, A-70171
Cyclohepta[*b*]pyrrol-2(1*H*)-one; *N*-Ac, *in* C-60201
2-Nitrobicyclo[4.4.1]undeca-1,3,5,7,9-pentaene, N-80038
3-Nitrobicyclo[4.4.1]undeca-1,3,5,7,9-pentaene, N-80039

$C_{11}H_9NO_2S$
2-Amino-3-(methylthio)-1,4-naphthalenedione, *in* A-70163

$C_{11}H_9NO_3$
2-Formyl-1*H*-indole-3-acetic acid, F-80075
2-Oxo-2*H*-benzopyran-4-acetic acid; Amide, *in* O-60057
4-Oxo-4*H*-1-benzopyran-3-acetic acid; Amide, *in* O-60059
5-Phenyl-4-oxazolecarboxylic acid; Me ester, *in* P-80112

$C_{11}H_9NO_4$
5-Methoxy-4-nitro-1-naphthol, *in* N-80054
6-Methoxy-1-nitro-2-naphthol, *in* N-80048

$C_{11}H_9N_2^{\oplus}$
Dipyrido[1,2-*a*:1′,2′-*c*]imidazol-10-ium(1+), D-70501

$C_{11}H_9N_3$
▷ 2-Amino-α-carboline, A-70105
3-Amino-α-carboline, A-70106
4-Amino-α-carboline, A-70107
6-Amino-α-carboline, A-70108
1-Amino-β-carboline, A-70109
3-Amino-β-carboline, A-70110
4-Amino-β-carboline, A-70111
6-Amino-β-carboline, A-70112
8-Amino-β-carboline, A-70113
8-Amino-δ-carboline, A-70119
1-Amino-γ-carboline, A-70114
3-Amino-γ-carboline, A-70115
5-Amino-γ-carboline, A-70116
6-Amino-γ-carboline, A-70117
8-Amino-γ-carboline, A-70118
1-Methyl-8*H*-benzo[*cd*]triazirino[*a*]indazole, M-60052
2-Methyl-2*H*-naphtho[1,8-*de*]triazine, M-70095
10*H*-Pyrazolo[5,1-*c*][1,4]benzodiazepine, P-70154
9*H*-Pyrrolo[1,2-*a*]indol-9-one; Hydrazone, *in* P-60247

$C_{11}H_9N_3O$
3,5-Dihydro-4*H*-pyrazolo[3,4-*c*]quinolin-4-one; N^5-Me, *in* D-80245
Di-2-pyridyl ketone; Oxime, *in* D-70502
Di-3-pyridyl ketone; Oxime, *in* D-70503
Di-4-pyridyl ketone; Oxime, *in* D-70504
2-Pyridyl 3-pyridyl ketone; Oxime, *in* P-70179
2-Pyridyl 4-pyridyl ketone; Oxime, *in* P-70180
3-Pyridyl 4-pyridyl ketone; Oxime, *in* P-70181

$C_{11}H_9N_3O_3$
8-Amino-6-nitroquinoline; 8-*N*-Ac, *in* A-60235

$C_{11}H_9N_4^{\oplus}$
3-Phenyltetrazolo[1,5-*a*]pyridinium, P-60134

$C_{11}H_9N_5O$
2-Amino-1,7-dihydro-7-phenyl-6*H*-purin-6-one, A-70133

$C_{11}H_{10}$
1,4-Dihydro-1,4-methanonaphthalene, D-60256

$C_{11}H_{10}ClN_2O^{\oplus}$
1′-(Chlorocarbonyl)-1′,2′-dihydro-1,2′-bipyridinium (1+), C-80045

$C_{11}H_{10}Cl_2N_2O$
Phosgene-in-a-can, *in* C-80045

$C_{11}H_{10}IN_3$
6*H*-Dipyrido[1,2-*a*:2′,1′-*d*][1,3,5]triazin-5-ium; Iodide, *in* D-60495

$C_{11}H_{10}N_2$
3,4-Dihydro-β-carboline, D-60209
Di-2-pyridylmethane, D-60496

2-Methyl-4-phenylpyrimidine, M-70111
2-Methyl-5-phenylpyrimidine, M-70112
4-Methyl-2-phenylpyrimidine, M-70113
4-Methyl-5-phenylpyrimidine, M-70114
4-Methyl-6-phenylpyrimidine, M-70115
5-Methyl-2-phenylpyrimidine, M-70116
5-Methyl-4-phenylpyrimidine, M-70117

$C_{11}H_{10}N_2O$
1-Acetylisoquinoline; Oxime, *in* A-60039
4-Acetylisoquinoline; Oxime, *in* A-60041
2-Acetylquinoline; Oxime, *in* A-60049
5-Acetylquinoline; Oxime, *in* A-60052
6-Acetylquinoline; Oxime, *in* A-60053
7-Acetylquinoline; Oxime, *in* A-60054
8-Acetylquinoline; Oxime, *in* A-60055
3,4-Dihydro-β-carboline; 2-Oxide, *in* D-60209
4-Methoxy-2,2′-bipyridine, *in* H-80121
5-Methoxy-2,2′-bipyridine, *in* H-80123
6-Methoxy-3,4′-bipyridine, *in* H-80130
1-Methyl-2-phenyl-1*H*-imidazole-4-carboxaldehyde, *in* P-60111
1-Methyl-2-phenyl-1*H*-imidazole-5-carboxaldehyde, *in* P-60111
2-Methyl-4-phenylpyrimidine; 1-Oxide, *in* M-70111
4-Methyl-5-phenylpyrimidine; 1-Oxide, *in* M-70114
4-Methyl-5-phenylpyrimidine; 3-Oxide, *in* M-70114
4-Methyl-6-phenylpyrimidine; 1-Oxide, *in* M-70115
4-Methyl-6-phenylpyrimidine; 3-Oxide, *in* M-70115
5-Methyl-4-phenylpyrimidine; 1-Oxide, *in* M-70117
5-Methyl-4-phenylpyrimidine; 3-Oxide, *in* M-70117
5-Methyl-3(2*H*)-pyridazinone; 2-Ph, *in* M-70126
6-Methyl-3-pyridazinone; 2-Ph, *in* M-70124

$C_{11}H_{10}N_2OS_2$
Spirobrassinin, S-60041

$C_{11}H_{10}N_2O_2$
5-Amino-3-phenylisoxazole; *N*-Ac, *in* A-60240
3-Amino-2(1*H*)-quinolinone; 3-*N*-Ac, *in* A-60256
4-Hydroxy-2,2′-bipyridine; Me ether, *N*-oxide, *in* H-80121
3-Hydroxy-3′-methoxy-2,2′-bipyridine, *in* D-80290
4-Methoxy-2,2′-bipyridin-6-ol, *in* D-80296
5-Methyl-4-phenylpyrimidine; 1,3-Dioxide, *in* M-70117

$C_{11}H_{10}N_2O_3$
4-Hydroxy-2,2′-bipyridine; Me ether, *N,N′*-dioxide, *in* H-80121

$C_{11}H_{10}N_3^{\oplus}$
6*H*-Dipyrido[1,2-*a*:2′,1′-*d*][1,3,5]triazin-5-ium, D-60495

$C_{11}H_{10}N_4$
5-Amino-1-benzyl-4-cyanopyrazole, *in* A-70192

$C_{11}H_{10}N_4O_2$
lin-Benzotheophylline, *in* I-60009

$C_{11}H_{10}O$
2-Acetyl-1*H*-indene, A-70045
3-Acetyl-1*H*-indene, A-70046
6-Acetyl-1*H*-indene, A-70047
Hexacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}.0^{8,11}]undecan-4-one, H-60035
2-Naphthalenemethanol, N-60004
2,3,5,6-Tetramethylenebicyclo[2.2.1]heptan-7-one, T-70136

$C_{11}H_{10}O_2$
2,5-Dimethyl-4*H*-1-benzopyran-4-one, D-70371
6-Methoxy-5-vinylbenzofuran, *in* H-70231
2-Methyl-1,3-naphthalenediol, M-60091
2-Methyl-1,5-naphthalenediol, M-60092
3-Methyl-1,2-naphthalenediol, M-60093
4-Methyl-1,3-naphthalenediol, M-60094
6-Methyl-1,2-naphthalenediol, M-60095
5-(2-Methyloxiranyl)benzofuran, M-70101
Pentacyclo[6.2.1.0^{2,7}.0^{4,10}.0^{5,9}]undecane-3,6-dione, P-70022
5-Phenyl-2,4-pentadienoic acid, P-70086

$C_{11}H_{10}O_2S$
5-(5-Methyl-2-thienyl)-2-penten-4-ynoic acid; Me ester, *in* M-80162
4-Methylthio-2,4-decadiene-6,8-diynoic acid, M-80163
5-Methylthio-2,4-decadiene-6,8-diynoic acid, M-80164
7-Methylthio-2,6-decadiene-4,8-diynoic acid, M-80165
7-Methylthio-2,6-decadiene-4,8-diynoic acid, M-80166
9-Methylthio-2,8-decadiene-4,6-diynoic acid, M-80167
5-(3-Methylthio-2-hexen-4-ynylidene)-2(5*H*)-furanone, M-80171
5-(5-Methylthio-4-hexen-2-ynylidene)-2(5*H*)-furanone, M-80172
6-[4-(Methylthio)-1,2,3-pentatrienyl]-2*H*-pyran-2-one, M-80174
6-[4-(Methylthio)-1,2,3-pentatrienyl]-2*H*-pyran-2-one; 1′,2′-Didehydro, 2′,3′-dihydro (*Z*-), *in* M-80174

$C_{11}H_{10}O_3$
7-Hydroxy-3,4-dimethyl-2*H*-1-benzopyran-2-one, H-60119
8-Methoxy-4-methyl-2*H*-1-benzopyran-2-one, *in* H-70165
5-Methoxy-4-methylcoumarin, *in* H-60173

$C_{11}H_{10}O_4$
2,3-Dihydro-3,5-dihydroxy-2-methylnaphthoquinone, D-70191
▷ 6,7-Dimethoxy-2*H*-1-benzopyran-2-one, *in* D-84287
8,13-Dioxapentacyclo[6.5.0.0^{2,6}.0^{5,10}.0^{3,11}]tridecane-9,12-dione, D-60467
3-Ethyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one, E-70040
7-Hydroxy-4-methoxy-5-methyl-2*H*-1-benzopyran-2-one, *in* D-60348
6-(Hydroxymethyl)-7-methoxy-2*H*-1-benzopyran-2-one, *in* H-70139
3-(2-Methoxy-4,5-methylenedioxyphenyl)propenal, M-70048
Methyl 3-benzoyloxyacrylate, *in* O-60090
Murrayacarpin A, M-80198

$C_{11}H_{10}O_5$
Benzyl hydrogen 2-formylmalonate, *in* H-80204
2,7-Dihydroxy-2,4,6-cycloheptatrien-1-one; Di-Ac, *in* D-60314
5-Hydroxy-6,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287
7-Hydroxy-5,6-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287
8-Hydroxy-5,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80288
Mandshurin, *in* T-80287

$C_{11}H_{10}O_6$
6-Hydroxy-5,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287

$C_{11}H_{11}BrN_2O_2$
2-Bromotryptophan, B-60332
5-Bromotryptophan, B-60333
6-Bromotryptophan, B-60334
7-Bromotryptophan, B-60335

$C_{11}H_{11}ClN_2O_2$
2-Chlorotryptophan, C-60145
6-Chlorotryptophan, C-60146

$C_{11}H_{11}Cl_2NO_2$
4,6-Dichloro-5-[(dimethylamino)methylene]-3,6-cyclohexadiene-1,3-dicarboxaldehyde, D-70119

$C_{11}H_{11}F_4O_2$
2,3,5,6-Tetrafluorobenzaldehyde; Di-Et acetal, *in* T-70028

$C_{11}H_{11}N$
2-Benzylpyrrole, B-80060
3-Benzylpyrrole, B-80061
▷ 2-Methyl-5-phenyl-1*H*-pyrrole, M-60115
3-(2-Propenyl)indole, P-60183
1,2,3,4-Tetrahydrocyclopent[*b*]indole, T-70049

$C_{11}H_{11}NO$
1,3-Dimethyl-1*H*-indole-2-carboxaldehyde, *in* M-70090
2,4-Dimethyl-5-phenyloxazole, D-80469
1-(2-Furanyl)-2-(2-pyrrolyl)ethylene; *N*-Me, *in* F-60088
3*a*,7*a*-Methano-1*H*-indole; *N*-Ac, *in* M-70041
1-(4-Methoxyphenyl)pyrrole, *in* H-60216
2-(2-Methoxyphenyl)pyrrole, *in* H-60217

$C_{11}H_{11}NO_2$
3,3-Dimethyl-2,4(1*H*,3*H*)-quinolinedione, D-60451
1*H*-Indole-3-acetic acid; *N*-Me, *in* I-70013
1*H*-Indole-3-carboxylic acid; Et ester, *in* I-80012
1-Methyl-3-phenyl-2,5-pyrrolidinedione, *in* P-80132

$C_{11}H_{11}NO_2S$
α-Aminobenzo[*b*]thiophene-3-acetic acid; Me ester, *in* A-60090
3-Amino-2-benzo[*b*]thiophenecarboxylic acid; Et ester, *in* A-60091

$C_{11}H_{11}NO_3$
3-Aminodihydro-2(3*H*)-furanone; *N*-Benzoyl, *in* A-60138
3-Amino-4-hydroxybutanoic acid; Lactone, *N*-benzoyl, *in* A-80081
2,3-Dihydro-2-oxo-1*H*-indole-3-acetic acid; Me ester, *in* D-60259
Methyl 2-formyl-3-phenylamino-2-propenoate, *in* A-80134
3-Morpholinone; 4-Benzoyl, *in* M-60147
1,2,3,4-Tetrahydro-2-oxo-4-quinolinecarboxylic acid; Me ester, *in* T-60077
1,2,3,4-Tetrahydro-4-oxo-6-quinolinecarboxylic acid; Me ester, *in* T-60078

$C_{11}H_{11}NO_4$
5,6-Dihydroxy-1*H*-indole-2-carboxylic acid; Di-Me ether, *in* D-70308
5,6-Dihydroxy-1*H*-indole-2-carboxylic acid; Et ester, *in* D-70308

$C_{11}H_{11}NO_7$
4-Hydroxy-5-nitro-1,2-benzenedicarboxylic acid; Me ether, di-Me ester, *in* H-70191
4-Hydroxy-5-nitro-1,3-benzenedicarboxylic acid; Me ether, di-Me ester, *in* H-70192

$C_{11}H_{11}NS$
1-(2-Pyrrolyl)-2-(2-thienyl)ethylene; *N*-Me, *in* P-60250

$C_{11}H_{11}N_3O_2$
3-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Benzyl, *in* A-70187
4,5-Dihydro-5,5-dimethyl-3*H*-1,2,4-triazol-3-one; *N*-Benzoyl, *in* D-80196
Methyl 1-benzyl-1*H*-1,2,3-triazole-5-carboxylate, *in* T-60239
2-Phenyl-2*H*-1,2,3-triazole-4-carboxylic acid; Et ester, *in* P-60140
1*H*-1,2,3-Triazole-4-carboxylic acid; 1-Benzyl, Me ester, *in* T-60239

$C_{11}H_{11}N_3O_4$
2-Nitrotryptophan, N-70067

$C_{11}H_{11}O_2^{\oplus}$
4,5-Dimethyl-2-phenyl-1,3-dioxol-1-ium, D-70431

$C_{11}H_{12}$
Benzylidenecyclobutane, B-70081
3-Cycloundecene-1,5-diyne, C-80201
1,4-Methano-1,2,3,4-tetrahydronaphthalene, M-60034
1-Phenyl-1,2-pentadiene, P-70085
3-Phenyl-1-pentyne, P-70089
4,5,6,7-Tetrahydro-1*H*-cyclopropa[*a*]naphthalene, T-70051
3,4,5,6-Tetrahydro-1*H*-cyclopropa[*b*]naphthalene, T-70050

1,2,3,4-Tetrahydro-1-methylenenaphthalene, T-60073
Tricyclo[5.4.0.0^{2,8}]undeca-3,5,9-triene, T-80246

$C_{11}H_{12}Br_2N_2$
1,1′-Methylenebispyridinium(1+); Dibromide, *in* M-70065

$C_{11}H_{12}F_2N_2O_5$
5-(2,2-Difluorovinyl)-2′-deoxyuridine, *in* D-80167
5-(2,2-Difluorovinyl)uracil; 1-(2-Deoxy-α-D-ribofuranosyl), *in* D-80167

$C_{11}H_{12}I_2N_2$
1,1′-Methylenebispyridinium(1+); Diiodide, *in* M-70065

$C_{11}H_{12}N_2$
5-Amino-1-methylisoquinoline; *N*-Me, *in* A-80102
4,4-Dimethyl-2-phenyl-4*H*-imidazole, D-70432

$C_{11}H_{12}N_2^{\oplus}$
1,1′-Methylenebispyridinium(1+), M-70065

$C_{11}H_{12}N_2O$
5-Amino-3-phenylisoxazole; *N*-Et, *in* A-60240

$C_{11}H_{12}N_2O_2$
5-Oxo-2-pyrrolidinecarboxylic acid; Anilide, *in* O-70102

$C_{11}H_{12}N_2O_4$
2,4-Diaminobenzoic acid; 2,4-*N*-Di-Ac, *in* D-60032

$C_{11}H_{12}N_2O_5$
2′-Deoxy-5-ethynyluridine, *in* E-60060

$C_{11}H_{12}N_2O_6$
5-Ethynyluridine, *in* E-60060

$C_{11}H_{12}N_4O$
5-Amino-1-(phenylmethyl)-1*H*-pyrazole-4-carboxamide, *in* A-70192

$C_{11}H_{12}O$
2,4,6-Cycloheptatrien-1-ylcyclopropylmethanone, C-60206
2,3-Dihydro-2,2-dimethyl-1*H*-inden-1-one, D-60227
2-Methyl-4-phenyl-3-butyn-2-ol, M-70110
3-Phenylcyclopentanone, P-80099
1-Phenyl-3-penten-1-one, P-60127
5-Phenyl-4-penten-2-one, P-70088
1,2,3,4-Tetrahydro-7*H*-benzocyclohepten-7-one, T-60057

$C_{11}H_{12}OS$
2,3-Dihydro-2,2-dimethyl-4*H*-1-benzothiopyran, D-70193

$C_{11}H_{12}O_2$
8-Decene-4,6-diynoic acid; Me ester, *in* D-70018
3-Oxo-5-phenylpentanal, O-80092
4-Oxo-5-phenylpentanal, O-80093
5-Oxo-5-phenylpentanal, O-80094
2-Phenylcyclopropanecarboxylic acid; Me ester, *in* P-60087
1-Phenyl-1,2-pentanedione, P-80115
1-Phenyl-1,3-pentanedione, P-80116
1-Phenyl-1,4-pentanedione, P-80117
1-Phenyl-2,4-pentanedione, P-80118

$C_{11}H_{12}O_2S$
4-Mercapto-2-butenoic acid; Benzyl ester, *in* M-60018
5-Methylthio-2,4,8-decatrien-6-ynoic acid, M-80168
3-[(4-Methylthio)phenyl]-2-butenoic acid, M-80179
2-[2-(Methylthio)propenyl]benzoic acid, M-80182
4-[2-(Methylthio)propenyl]benzoic acid, M-80183

$C_{11}H_{12}O_3$
Asperpentyne, A-80179
3-Benzoyl-2-methylpropanoic acid, B-60064
3,4-Dihydro-2*H*-1-benzopyran-2-ol; Ac, *in* D-60198
3,4-Dihydro-2*H*-1-benzopyran-4-ol; Ac, *in* D-60200
3,4-Dihydro-2*H*-1-benzopyran-6-ol; Ac, *in* D-70175
3-(4-Hydroxyphenyl)-2-propenoic acid; Et ester, *in* H-80242
3-(4-Hydroxy-2-vinylphenyl)propanoic acid, H-70232
1,2,3,4-Tetrahydro-1-hydroxy-2-naphthalenecarboxylic acid, T-70063

$C_{11}H_{12}O_4$
1,3,5-Cycloheptatriene-1,6-dicarboxylic acid; Di-Me ester, *in* C-60202
5,7-Dimethoxy-6-methylphthalide, *in* D-60349
4-Hydroxybenzyl alcohol; Di-Ac, *in* H-80114
Pyrenocine A, P-80203

$C_{11}H_{12}O_5$
2-Formyl-3,5-dihydroxybenzoic acid; Di-Me ether, Me ester, *in* F-60071
5-Hydroxy-3-methyl-1,2-benzenedicarboxylic acid; Me ether, 2-Me ester, *in* H-70162

$C_{11}H_{12}O_6$
3-Oxotricyclo[2.1.0.0^{2,5}]pentane-1,5-dicarboxylic acid; Di-Me ester, ethylene ketal, *in* O-80096

$C_{11}H_{12}S$
2,2-Dimethyl-2*H*-1-benzothiopyran, D-70373

$C_{11}H_{12}S_2$
2-(2,4,6-Cycloheptatrien-1-ylidene)-1,3-dithiane, C-70221

$C_{11}H_{13}BrN_2O_5$
5-(2-Bromovinyl)-2′-deoxyuridine, B-80266

$C_{11}H_{13}BrO_2$
3-Bromo-2,4,6-trimethylbenzoic acid; Me ester, *in* B-60331

$C_{11}H_{13}IO_4$
2,5-Dihydroxy-4-iodobenzoic acid; Di-Me ether, Et ester, *in* D-60333

$C_{11}H_{13}I_2NO$
2,6-Diiodobenzoic acid; Diethylamide, *in* D-70356

$C_{11}H_{13}N$
1,2,3,6-Tetrahydro-4-phenylpyridine, T-60081
1,2,3,6-Tetrahydropyridine; 1-Ph, *in* T-70089

$C_{11}H_{13}NO$
3,4-Dihydro-3,3-dimethyl-2(1*H*)quinolinone, D-60231
3-Isopropyloxindole, I-70097
4-(Phenylimino)-2-pentanone, *in* P-60059
1,2,3,4-Tetrahydroquinoline; *N*-Ac, *in* T-70093

$C_{11}H_{13}NO_2$
2-Amino-3-phenyl-3-butenoic acid; Me ester, *in* A-60238
5,6-Dihydroxyindole; Di-Me ether, *N*-Me, *in* D-70307
1,2,3,4-Tetrahydro-4-hydroxyisoquinoline; *N*-Ac, *in* T-60066
1,2,3,4-Tetrahydro-3-methyl-3-isoquinolinecarboxylic acid, T-60074
5-(3,4,5,6-Tetrahydro-3-pyridylidenemethyl)-2-furanmethanol, T-60087

$C_{11}H_{13}NO_3$
1-Amino-2-(4-hydroxyphenyl)cyclopropanecarboxylic acid; Me ester, *in* A-60197
1-Amino-2-(4-hydroxyphenyl)cyclopropanecarboxylic acid; Me ether, *in* A-60197
Ethyl *N*-phenacylcarbamate, *in* O-70099
2,3,4-Trihydroxyphenylacetic acid; Tri-Me ether, nitrile, *in* T-60340
2,4,5-Trihydroxyphenylacetic acid; Tri-Me ether, nitrile, *in* T-60342
▷ 3,4,5-Trimethoxybenzeneacetonitrile, *in* T-60343

$C_{11}H_{13}NO_4$
2-Amino-2-benzylbutanedioic acid, A-60094
2-Amino-4-hydroxybutanoic acid; *N*-Benzoyl, *in* A-70156
2-Amino-3-phenylpentanedioic acid, A-60241
2,6-Bis(methoxyacetyl)pyridine, *in* B-70144
(±)-Isothreonine; *N*-Benzoyl, *in* A-60183
3,5-Pyridinedipropanoic acid, P-60217
Threonine; *N*-Benzoyl, *in* T-60217

$C_{11}H_{13}NO_5$
5-Amino-4-hydroxy-1,3-benzenedicarboxylic acid; Me ether, di-Me ester, *in* A-70155
Dimethyl 4-amino-5-methoxyphthalate, *in* A-70152

$C_{11}H_{13}N_3O_4$
2′-Deoxy-5-ethynylcytidine, *in* A-60153
Imidazo[4,5-*c*]pyridine; 1-β-D-Ribofuranosyl, *in* I-60008

$C_{11}H_{13}N_3O_5$
5-Ethynylcytidine, *in* A-60153

$C_{11}H_{14}$
6-(1,3-Butadienyl)-1,4-cycloheptadiene, B-70290
2-Phenyl-2-pentene, P-80119

$C_{11}H_{14}N_2$
5,6,9,10-Tetrahydro-4*H*,8*H*-pyrido[3,2,1-*ij*][1,6]naphthyridine, T-60086

$C_{11}H_{14}N_2O$
Piperazinone; N^4-Benzyl, *in* P-70101

$C_{11}H_{14}N_2O_3$
2,4,6-Trimethyl-3-nitroaniline; *N*-Ac, *in* T-70285

$C_{11}H_{14}N_2O_4$
4-Amino-2,6-pyridinedicarboxylic acid; Di-Et ester, *in* A-70194

$C_{11}H_{14}N_2O_5$
2′-Deoxy-5-vinyluridine, *in* V-70015

$C_{11}H_{14}N_2O_6$
2-Amino-3,5-pyridinedicarboxylic acid; Di-Et ester, *in* A-70193
5-Vinyluridine, V-70015

$C_{11}H_{14}N_4$
4-(Butylimino)-3,4-dihydro-1,2,3-benzotriazine(incorr.), *in* A-60092

$C_{11}H_{14}N_4O_3$
4-Amino-1*H*-imidazo[4,5-*c*]pyridine; 1-(2-Deoxy-β-D-ribofuranosyl), *in* A-70161
4-Amino-1*H*-imidazo[4,5-*c*]pyridine; 1-(5-Deoxy-β-D-ribofuranosyl), *in* A-70161

$C_{11}H_{14}N_4O_3S$
2′-Deoxy-7-deaza-6-thioguanosine, *in* A-80144

$C_{11}H_{14}N_4O_4$
4-Amino-4,6-dihydro-3-methyl-1*H*-cyclopenta[*e*]1,2,4-triazine-5,7-dicarboxylic acid; Di-Me ester, *in* A-80066
4-Amino-1*H*-imidazo[4,5-*c*]pyridine; 1-β-D-Ribofuranosyl, *in* A-70161
1-Deazaadenosine, *in* A-80087
7-Deaza-2′-deoxyguanosine, *in* A-60255
2-Methyl-9-β-D-ribofuranosyl-9*H*-purine, M-70130
6-Methyl-9-β-D-ribofuranosyl-9*H*-purine, M-70131

$C_{11}H_{14}N_4O_4S$
▷ 6-(Methylthio)-9-β-D-ribofuranosyl-9*H*-purine, *in* T-70180

$C_{11}H_{14}N_4O_5$
7-Deazaguanosine, *in* A-60255

$C_{11}H_{14}O$
3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran, D-80184
2,2-Dimethyl-1-phenyl-1-propanone, D-60443
(3-Hydroxyphenoxy)acetic acid; Me ether, Et ester, *in* H-70204
4-Methoxy-4-phenyl-1-butene, *in* P-70061
3-Methyl-2-phenylbutanal, M-70109
Spiro[5.5]undeca-1,3-dien-7-one, S-60046

$C_{11}H_{14}O_2$
Andirolactone, A-60271
1,1′-Bi(bicyclo[1.1.1]pentane)-3-carboxylic acid, B-80072

3-*tert*-Butyl-4-hydroxybenzaldehyde, B-70304
1-(Phenylmethoxy)-3-buten-2-ol, *in* B-70291
1,2,3,4-Tetrahydro-1-hydroxy-2-naphthalenemethanol, T-70064
Tricyclo[3.3.3.0^{1,5}]undecane-3,7-dione, T-80245
Tricyclo[4.3.1.1^{3,8}]undecane-2,7-dione, T-70233
Tricyclo[4.3.1.1^{3,8}]undecane-4,5-dione, T-70234
3,4,5-Trimethylbenzoic acid; Me ester, *in* T-60355
3,4,5-Trimethylphenol; Ac, *in* T-60371

$C_{11}H_{14}O_3$
1,2,3,4,5,6,7,8-Octahydro-8-oxo-2-naphthalenecarboxylic acid, O-80015

$C_{11}H_{14}O_4$
2-(3,4-Dihydroxyphenyl)propanoic acid; Di-Me ether, *in* D-60372
2,6-Dimethoxy-3,5-dimethylbenzoic acid, *in* D-70293
6-Ethyl-2,4-dihydroxy-3-methylbenzoic acid; Me ester, *in* E-70041
2′-Hydroxy-4′,6′-dimethoxy-3′-methylacetophenone, *in* T-80321
3-(4-Hydroxy-3,5-dimethoxyphenyl)propanal, *in* T-80333
3-Hydroxy-5-(4-hydroxyphenyl)pentanoic acid, H-70142
(2-Hydroxyphenoxy)acetic acid; Me ether, Et ester, *in* H-70203
(4-Hydroxyphenoxy)acetic acid; Me ether, Et ester, *in* H-70205
Pyrenocine C, *in* P-80203
Sinapyl alcohol, S-70046
2′,4′,6′-Trimethoxyacetophenone, *in* T-70248
3′,4′,5′-Trimethoxyacetophenone, *in* T-60315

$C_{11}H_{14}O_5$
Pyrenocine B, *in* P-80203
3,4,6-Trihydroxy-2-methylbenzoic acid; 4,6-Di-Me ether, Me ester, *in* T-80324
2,3,4-Trimethoxybenzeneacetic acid, *in* T-60340
2,4,5-Trimethoxybenzeneacetic acid, *in* T-60342
3,4,5-Trimethoxybenzeneacetic acid, *in* T-60343
3,4,6-Trimethoxy-2-methylbenzoic acid, *in* T-80324

$C_{11}H_{14}O_6$
2,3,5,6-Tetramethoxybenzoic acid, *in* T-60100
(3,4,5-Trihydroxy-6-oxo-1-cyclohexen-1-yl)methyl 2-butenoate, T-60338

$C_{11}H_{15}Br$
(Bromomethylidene)adamantane, B-60296
Bromopentamethylbenzene, B-60312

$C_{11}H_{15}Cl$
Chloropentamethylbenzene, C-60122

$C_{11}H_{15}N$
1-Amino-1-phenyl-4-pentene, A-70183
2-Methyl-5-phenylpyrrolidine, M-80147
2-Phenylcyclopentylamine, P-60086
[6](2,6)Pyridinophane, P-80211
2,3,4,5-Tetrahydro-1*H*-1-benzazepine; 1-Me, *in* T-70036

$C_{11}H_{15}NO$
1-Isocyanatoadamantane, I-80053
[6](2,6)Pyridinophane; *N*-Oxide, *in* P-80211

$C_{11}H_{15}NOS$
Tetrahydro-2-thiophenecarboxylic acid; Anilide, *in* T-70099
Tricyclo[3.3.1.1^{3,7}]decyl-1-sulfinylcyanide, *in* T-70177

$C_{11}H_{15}NO_2$
2-Amino-2-methyl-3-phenylpropanoic acid; Me ester, *in* A-60225
1,2,3,4,5-Pentamethyl-6-nitrobenzene, P-60057

$C_{11}H_{15}NO_2S$
2-Amino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylic acid; Et ester, *in* A-60258

$C_{11}H_{15}NO_3$
2-Amino-3-(4-hydroxyphenyl)-3-methylbutanoic acid, A-60198
4-Amino-3-hydroxy-5-phenylpentanoic acid, A-60199

$C_{11}H_{15}NO_4$
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid; Di-Me ester, *in* D-80193
3′,4′,5′-Trihydroxyacetophenone; Tri-Me ether, oxime, *in* T-60315

$C_{11}H_{15}NO_5$
3-Hydroxy-1*H*-pyrrole-2,4-dicarboxylic acid; Me ether, Di-Et ester, *in* H-80251
1*H*-Pyrrole-3,4-dicarboxylic acid; 1-Methoxy, di-Et ester, *in* P-70183

$C_{11}H_{15}NS$
3-Aminotetrahydro-2*H*-thiopyran; *N*-Ph, *in* A-70200
1-Thiocyanatoadamantane, T-70177

$C_{11}H_{15}N_5O$
1′-Methylzeatin, M-60133

$C_{11}H_{15}N_5O_3$
1-[3-Azido-4-(hydroxymethyl)cyclopentyl]-5-methyl-2,4(1*H*,3*H*)pyrimidinedione, A-70288

$C_{11}H_{15}N_5O_4$
Euglenapterin, E-60070

$C_{11}H_{15}N_5O_5$
Ara-doridosine, *in* A-60144
Doridosine, D-60518
1-Methylguanosine, M-70084
8-Methylguanosine, M-70085

$C_{11}H_{15}N_5O_5S$
8-(Methylthio)guanosine, *in* M-70029

$C_{11}H_{15}N_5O_6$
8-Methoxyguanosine, *in* D-70238

$C_{11}H_{15}N_5O_7S$
8-(Methylsulfonyl)guanosine, *in* M-70029

$C_{11}H_{16}$
Bicyclo[4.4.1]undeca-1,6-diene, B-70115
1-Cycloundecen-3-yne, C-70256
2,3-Dimethylenebicyclo[2.2.3]nonane, D-70406
2,6-Dimethylenebicyclo[3.3.1]nonane, D-80448
(2,2-Dimethylpropyl)benzene, D-60445
Methyleneadamantane, M-60068
Tetracyclo[4.4.1.0^{3,11}.0^{9,11}]undecane, T-60037
1,3-Undecadien-5-yne, U-80017
1,5-Undecadien-3 yne, U-80018
4,7-Undecadiyne, U-80019
2,4,6,8-Undecatetraene, U-70003

$C_{11}H_{16}N_2O_3$
2-Amino-3-nitrobenzyl alcohol; *N*-Et, Et ether, *in* A-80125

$C_{11}H_{16}N_2O_5$
▷ 2′-Deoxy-5-ethyluridine, *in* E-60054

$C_{11}H_{16}N_2O_6$
5-Ethyluridine, *in* E-60054

$C_{11}H_{16}N_6O_3$
3′-Amino-3′-deoxyadenosine; 3′*N*-Me, *in* A-70128

$C_{11}H_{16}N_6O_5$
8-(Methylamino)guanosine, *in* A-70150

$C_{11}H_{16}O$
5,6,7,8,9,10-Hexahydro-4*H*-cyclonona[*c*]furan, H-60047
1-Methyladamantanone, M-60040
5-Methyladamantanone, M-60041
3-Oxatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane, O-70069
Pentamethylphenol, P-60058
2,2,5,5-Tetramethylbicyclo[4.1.0]hept-1(6)-en-7-one, T-70131
2,4-Undecadiyn-1-ol, U-80020

$C_{11}H_{16}O_2$
Bicyclo[2.2.2]oct-2-ene-1-carboxylic acid; Et ester, *in* B-70113
1,3-Dimethoxy-1-phenylpropane, *in* P-80122
▷ 3,4-Dimethyl-5-pentylidene-2(5*H*)-furanone, D-70430
Spiro[5.5]undecane-1,9-dione, S-70066
Spiro[5.5]undecane-3,8-dione, S-70067
Spiro[5.5]undecane-3,9-dione, S-70068

$C_{11}H_{16}O_4$
Methylenolactocin, M-70079
1,2,3,4-Tetramethoxy-5-methylbenzene, *in* M-80050
▷ Xanthotoxol, X-60002

$C_{11}H_{16}O_5$
3,6-Dihydro-2*H*-pyran-2,2-dicarboxylic acid; Di-Et ester, *in* D-80243

$C_{11}H_{16}O_8$
Ranunculin, *in* H-60182

$C_{11}H_{17}N$
3-Azatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane, A-70282
Spiro[aziridine-2,2′-tricyclo[3.1.1.1^{3,7}]decane], S-80040

$C_{11}H_{17}NO_7$
2-(Dimethylamino)benzaldehyde; Di-Me acetal, *in* D-60401

$C_{11}H_{18}$
2,2-Dimethyl-3-methylenebicyclo[2.2.2]octane, D-60427
4,8-Dimethyl-1,3,7-nonatriene, D-50644
1,3,5-Undecatriene, U-70004

$C_{11}H_{18}N_2O_2$
Cyclo(leucylprolyl), C-80185
2-Diazo-2,2,6,6-tetramethyl-3,5-heptanedione, D-70064
Hexahydro-3-(1-methylpropyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, H-60052
Spiro[5.5]undecane-3,9-dione; Dioxime, *in* S-70068

$C_{11}H_{18}N_2O_3$
Cyclo(hydroxyprolylleucyl), C-60213

$C_{11}H_{18}O$
2-Cycloundecen-1-one, C-70255
2-Ethyl-4,6,6-trimethyl-2-cyclohexen-1-one, E-80068

$C_{11}H_{18}OS$
2-(Methylsulfinyl)adamantane, *in* A-80038

$C_{11}H_{18}O_2$
Bicyclo[2.2.2]octane-1-carboxylic acid; Et ester, *in* B-60092
3,3,4,4,5,5-Hexamethyl-1,2-cyclopentanedione, H-80074
2-Hexyl-5-methyl-3(2*H*)furanone, H-60079
1-Methoxy-3-myodesertene, *in* M-80203

$C_{11}H_{18}O_2S$
2-(Methylsulfonyl)adamantane, *in* A-80038

$C_{11}H_{18}O_3$
2,3-Di-*tert*-butoxycyclopropenone, *in* D-70290
Dihydro-3,3,4,4,5,5-hexamethyl-2*H*-pyran-2,6(3*H*)-dione, D-80210
Dihydro-3,3,4,4,5,5-hexamethyl-2*H*-pyran-2,6(3*H*)dione, *in* H-80076
1,3-Dihydroxy-4-methyl-6,8-decadien-5-one, D-70321
Queen substance; Me ester, *in* O-70089

$C_{11}H_{18}O_4$
Citreoviral, C-60150
Phaseolinic acid, P-60067

$C_{11}H_{18}O_5$
4-Oxoheptanedioic acid; Di-Et ester, *in* O-60071
4,4-Pyrandiacetic acid; Di-Me ester, *in* P-70150

$C_{11}H_{18}O_6$
Eccremocarpol A, E-80002

$C_{11}H_{18}S$
2-(Methylthio)adamantane, *in* A-80038

$C_{11}H_{19}NO_8$
Agropinic acid, A-70075

$C_{11}H_{19}N_3O_7$
Nitropeptin, N-70055

$C_{11}H_{20}$
Cycloundecene, C-80200
1,1,3,3-Tetramethyl-2-methylenecyclohexane, T-60144
1,10-Undecadiene, U-80008
1,2-Undecadiene, U-80003
1,3-Undecadiene, U-80004
1,4-Undecadiene, U-80005
1,5-Undecadiene, U-80006
1,6-Undecadiene, U-80007
2,3-Undecadiene, U-80009
2,4-Undecadiene, U-80010
2,5-Undecadiene, U-80011
2,9-Undecadiene, U-80012
3,5-Undecadiene, U-80013
4,6-Undecadiene, U-80014
4,7-Undecadiene, U-80015
5,6-Undecadiene, U-80016

$C_{11}H_{20}Br_2O$
1,11-Dibromo-6-undecanone, D-80107

$C_{11}H_{20}N_2$
3,4-Di-*tert*-butylpyrazole, D-70106
3,5-Di-*tert*-butylpyrazole, D-70107

$C_{11}H_{20}O$
10-Undecen-2-one, U-80022
5-Undecen-2-one, U-80023
10-Undecyn-2-ol, U-80032
1-Undecyn-5-ol, U-80024
3-Undecyn-1-ol, U-80025
4-Undecyn-1-ol, U-80026
4-Undecyn-2-ol, U-80027
5-Undecyn-1-ol, U-80028
5-Undecyn-2-ol, U-80029
6-Undecyn-1-ol, U-60004
6-Undecyn-5-ol, U-80030
7-Undecyn-1-ol, U-80031

$C_{11}H_{20}O_2$
2,7-Diethoxycycloheptene, *in* C-80179
1,1-Diethoxy-2-methylenecylohexane, *in* M-80080
2,4-Heptadienal; Di-Et acetal, *in* H-60020
2-Methyl-4-penten-1-ol; Tetrahydropyranyl ether, *in* M-80135

$C_{11}H_{20}O_3$
2-Hydroxycyclooctanecarboxylic acid; Et ester, *in* H-70121
2-Hydroxycyclooctanecarboxylic acid; Me ether, Me ester, *in* H-70121
10-Oxodecanoic acid; Me ester, *in* O-60063

$C_{11}H_{20}O_4$
Hexamethylpentanedioic acid, H-80076

$C_{11}H_{20}O_7$
Eccremocarpol B, E-80003

$C_{11}H_{21}Br$
11-Bromo-1-undecene, B-60336
1-Bromo-2-undecene, B-70277

$C_{11}H_{21}NO$
Hexahydro-5(2*H*)-azocinone; 1-*tert*-Butyl, *in* H-70048

$C_{11}H_{21}NO_3$
3-Oxocyclobutanecarboxylic acid; *N,N*-Dimethylamide, Di-Et ketal, *in* O-80073

$C_{11}H_{21}NO_9$
Mannopinic acid, M-70009

$C_{11}H_{21}NO_{10}S_3$
Glucoiberin, G-80022

$C_{11}H_{22}$
1,1-Di-*tert*-butylcyclopropane, D-60112

$C_{11}H_{22}N_2O$
4-Amino-2,2,6,6-tetramethylpiperidine; *N*-Ac, *in* A-70201

$C_{11}H_{22}N_2O_3$
N-Valylleucine, V-60001

$C_{11}H_{22}N_2O_8$
Mannopine, *in* M-70009

$C_{11}H_{22}O$
6-Undecen-1-ol, U-80021

$C_{11}H_{22}O_3$
2,2-Diethoxytetrahydro-5,6-dimethyl-2*H*-pyran, *in* T-70059
1,11-Dihydroxy-6-undecanone, D-80392
9-Hydroxydecanoic acid; Me ester, *in* H-80149
Sitophilate, *in* H-80209

$C_{11}H_{23}N$
Octahydroazocine; 1-*tert*-Butyl, *in* O-70010

$C_{11}H_{24}$
2,2,3,3,4,4-Hexamethylpentane, H-60071

$C_{11}H_{27}N_5$
1,4,7,10,13-Pentaazacyclohexadecane, P-60021

$C_{12}H_4Cl_4O_2$
▷ 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin, T-70016

$C_{12}H_4Cl_6$
▷ 2,2′,4,4′,5,5′-Hexachlorobiphenyl, H-60034

$C_{12}H_4S$
▷ Tetraethynylthiophene, T-80048

$C_{12}H_6$
▷ 1-Phenyl-1,3,5-hexatriyne, P-80105

$C_{12}H_6Br_2N_2O_4$
2,2′-Dibromo-3,5′-dinitrobiphenyl, D-80091
2,2′-Dibromo-5,5′-dinitrobiphenyl, D-80092
5,5′-Dibromo-2,2′-dinitrobiphenyl, D-80093

$C_{12}H_6Br_6$
Hexakis(bromomethylene)cyclohexane, H-80073

$C_{12}H_6Cl_2N_2$
1,4-Dichlorobenzo[*g*]phthalazine, D-70114

$C_{12}H_6Cl_2N_2O_2$
[2,2′-Bipyridine]-4,4′-dicarboxylic acid; Dichloride, *in* B-60126
[2,2′-Bipyridine]-6,6′-dicarboxylic acid; Dichloride, *in* B-60128

$C_{12}H_6Cl_4N_2O_4$
Pyrroxamycin, P-70203

$C_{12}H_6Cl_4O$
Bis(2,4-dichlorophenyl)ether, B-70135
Bis(2,6-dichlorophenyl) ether, B-70136
Bis(3,4-dichlorophenyl) ether, B-70137

$C_{12}H_6Cl_{12}$
Hexakis(dichloromethyl)benzene, H-60067

$C_{12}H_6F_2N_2O_4$
3,3′-Difluoro-4,4′-dinitrobiphenyl, D-80161
4,4′-Difluoro-2,2′-dinitrobiphenyl, D-80162
5,5′-Difluoro-2,2′-dinitrobiphenyl, D-80163

$C_{12}H_6I_2N_2O_4$
2,2′-Diiodo-4,5′-dinitrobiphenyl, D-80401
2,2′-Diiodo-5,5′-dinitrobiphenyl, D-80402
2,2′-Diiodo-6,6′-dinitrobiphenyl, D-80403
4,4′-Diiodo-3,3′-dinitrobiphenyl, D-80404

$C_{12}H_6N_2$
5,7-Dicyanoazulene, *in* A-70295
2,3-Dicyanonaphthalene, *in* N-80001

$C_{12}H_6N_2O_2$
Benzo[*g*]quinazoline-6,9-dione, B-60044
Benzo[*g*]quinoxaline-6,9-dione, B-60046
1,7-Phenanthroline-5,6-dione, P-70052

$C_{12}H_6N_2O_4$
1,5-Dinitrobiphenylene, D-80492
2,6-Dinitrobiphenylene, D-80493

$C_{12}H_6N_4$
5,5′-Dicyano-2,2′-bipyridine, *in* B-60127
Pyrazino[2′,3′:3,4]cyclobuta[1,2-*g*]quinoxaline, P-60198
1,2,4,5-Tetracyano-3,6-dimethylbenzene, *in* D-60407

$C_{12}H_6O_2S$
Naphtho[2,3-*b*]thiophene-2,3-dione, N-70014

$C_{12}H_6O_3$
Naphtho[2,3-*c*]furan-1,3-dione, *in* N-80001

$C_{12}H_6O_4$
2,2-Bi(1,4-benzoquinone), B-80069
4,4′-Bi(1,2-benzoquinone), B-80070

$C_{12}H_7Br$
1-Bromobiphenylene, B-80181
2-Bromobiphenylene, B-80182

$C_{12}H_7BrN_2$
2-Bromo-1,10-phenanthroline, B-70264
8-Bromo-1,7-phenanthroline, B-70265

$C_{12}H_7BrO_4$
2-Bromo-5-hydroxy-1,4-naphthoquinone; Ac, *in* B-60269
2-Bromo-6-hydroxy-1,4-naphthoquinone; Ac, *in* B-60270
2-Bromo-8-hydroxy-1,4-naphthoquinone; Ac, *in* B-60272

$C_{12}H_7ClN_2$
1-Chlorobenzo[*g*]phthalazine, C-70054

$C_{12}H_7ClN_2O$
4-Chlorobenzo[*g*]phthalazin-1(2*H*)-one, C-70055

$C_{12}H_7I$
1-Iodobiphenylene, I-80020
2-Iodobiphenylene, I-80021

$C_{12}H_7NOS$
1*H*-Phenothiazin-1-one, P-60078

$C_{12}H_7NO_2$
1*H*-Benz[*e*]indole-1,2(3*H*)-dione, B-70026
10*H*-[1]Benzopyrano[3,2-*c*]pyridin-10-one, B-60042
10*H*-[1]Benzopyrano[3,2-*c*]pyridin-10-one, B-80038
1*H*-Carbazole-1,4(9*H*)-dione, C-60012
3-Cyano-2-naphthoic acid, *in* N-80001
2*H*-Naphtho[2,3-*c*]pyrrole-1,3-dione, *in* N-80001
1-Nitrobiphenylene, N-80040
2-Nitrobiphenylene, N-80041

$C_{12}H_7NO_3$
2-Hydroxy-3*H*-phenoxazin-3-one, H-60206

$C_{12}H_7N_5$
7*H*-2,3,4,6,7-Pentaazabenz[*de*]anthracene, P-60017

$C_{12}H_8$
1-Ethylnylnaphthalene, E-70046

$C_{12}H_8ClNO$
1-Chloromethylbenz[*cd*]indol-2(1*H*)-one, *in* B-70027

$C_{12}H_8ClNOS$
3-Chloro-10*H*-phenothiazine; 5-Oxide, *in* C-60126
4-Chloro-10*H*-phenothiazine; 5-Oxide, *in* C-60127

$C_{12}H_8ClNO_2$
2-Chloro-7-nitro-9*H*-fluorene, C-70133
9-Chloro-2-nitro-9*H*-fluorene, C-70134
9-Chloro-3-nitro-9*H*-fluorene, C-70135

$C_{12}H_8ClNO_2S$
3-Chloro-10*H*-phenothiazine; 5,5-Dioxide, *in* C-60126
4-Chloro-10*H*-phenothiazine; 5,5-Dioxide, *in* C-60127

$C_{12}H_8ClNO_3$
▷ 2-Amino-3-chloro-1,4-naphthoquinone; *N*-Ac, *in* A-70122

$C_{12}H_8ClNS$
1-Chloro-10*H*-phenothiazine, C-60124
▷ 2-Chloro-10*H*-phenothiazine, C-60125
3-Chloro-10*H*-phenothiazine, C-60126

$C_{12}H_8Cl_2$
5,6-Dichloroacenaphthene, D-60115

$C_{12}H_8F_3NO_3$
7-Amino-4-(trifluoromethyl)-2*H*-1-benzopyran-2-one; *N*-Ac, *in* A-60265

$C_{12}H_8N_2$
Benzo[*c*]cinnoline, B-60020

Benzo[*b*]-[1,5]-naphthyridine, B-80030
Benzo[*b*][1,7]naphthyridine, B-80031
Benzo[*b*][1,8]naphthyridine, B-80032
Benzvalenoquinoxaline, B-70080

$C_{12}H_8N_2O$
Benzo[*c*]cinnoline; *N*-Oxide, *in* B-60020
2-(2-Furanyl)quinoxaline, F-60089

$C_{12}H_8N_2O_2$
▷ 2-Amino-3*H*-phenoxazin-3-one, A-60237
1*H*-Benz[*e*]indole-1,2(3*H*)-dione; 1-Oxime, *in* B-70026
Benzo[*c*]cinnoline; 5,6-Di-*N*-oxide, *in* B-60020
6,6′-(1,2-Ethynediyl)bis-2(1*H*)-pyridinone, E-80069

$C_{12}H_8N_2O_4$
[2,2′-Bipyridine]-3,3′-dicarboxylic acid, B-60124
[2,2′-Bipyridine]-3,5′-dicarboxylic acid, B-60125
[2,2′-Bipyridine]-4,4′-dicarboxylic acid, B-60126
[2,2′-Bipyridine]-5,5′-dicarboxylic acid, B-60127
[2,2′-Bipyridine]-6,6′-dicarboxylic acid, B-60128
[2,3′-Bipyridine]-2,3′-dicarboxylic acid, B-60129
[2,4′-Bipyridine]-2′,6′-dicarboxylic acid, B-60130
[2,4′-Bipyridine]-3,3′-dicarboxylic acid, B-60131
[2,4′-Bipyridine]-3′,5-dicarboxylic acid, B-60132
[3,3′-Bipyridine]-2,2′-dicarboxylic acid, B-60133
[3,3′-Bipyridine]-4,4′-dicarboxylic acid, B-60134
[3,4′-Bipyridine]-2′,6′-dicarboxylic acid, B-60135
[4,4′-Bipyridine]-2,2′-dicarboxylic acid, B-60136
[4,4′-Bipyridine]-3,3′-dicarboxylic acid, B-60137
2,2′-Dinitrobiphenyl, D-60460

$C_{12}H_8N_4$
Pyrido[1″,2″:1′,2′]imidazo[4′,5′:4,5]imidazo[1,2-*a*]pyridine, P-70175
Pyrido[2″,1″:2′,3′]imidazo[4′,5′:4,5]imidazo[1,2-*a*]pyridine, P-60234

$C_{12}H_8N_{10}O_{12}$
3,3′,5,5′-Tetraamino-2,2′,4,4′,6,6′-hexanitrobiphenyl, T-60014

$C_{12}H_8O$
Cyclobuta[*b*]naphthalen-1(2*H*)-one, C-80175
6*b*,7*a*-Dihydroacenaphth[1,2-*b*]oxirene, D-70170
4-Hydroxyacenaphthylene, H-70100
Naphtho[1,2-*c*]furan, N-70008
Naphtho[2,3-*c*]furan, N-60008
Naphtho[1,8-*bc*]pyran, N-70009
1-Phenyl-1,4-hexadiyn-3-one, P-60108
▷ 1-Phenyl-2,4-hexadiyn-1-one, P-60109
6-Phenyl-3,5-hexadiyn-2-one, P-60110

$C_{12}H_8OS$
4-Phenylthieno[3,4-*b*]furan, P-60135

$C_{12}H_8OSe$
Phenoxaselenin, P-80087

$C_{12}H_8O_2$
1,2-Biphenylenediol, B-80116
1,5-Biphenylenediol, B-80117
1,8-Biphenylenediol, B-80118
2,3-Biphenylenediol, B-80119
2,6-Biphenylenediol, B-80120
2,7-Biphenylenediol, B-80121
1,2-Dihydrocyclobuta[*a*]naphthalene-3,4-dione, D-60213
1,2-Dihydrocyclobuta[*b*]naphthalene-3,8-dione, D-60214
6-Hydroxy-1-phenyl-2,4-hexadiyn-1-one, H-80235
1,2-Naphthalenedicarboxaldehyde, N-60001
1,3-Naphthalenedicarboxaldehyde, N-60002

$C_{12}H_8O_2Se$
Phenoxaselenin; Se-Oxide, *in* P-80087

$C_{12}H_8O_2Se_2$
Selenanthrene; 9,10-Dioxide, *in* S-80021

$C_{12}H_8O_3$
2-Hydroxy-6-(2,4-pentadiynyl)benzoic acid, H-80231
α-Oxo-1-naphthaleneacetic acid, O-60078
α-Oxo-2-naphthaleneacetic acid, O-60079

$C_{12}H_8O_4$
1,4-Azulenedicarboxylic acid, A-70293
2,6-Azulenedicarboxylic acid, A-70294
5,7-Azulenedicarboxylic acid, A-70295
2,3-Naphthalenedicarboxylic acid, N-80001
β-Sorigenin, S-80039
▷ Xanthotoxin, X-60001

$C_{12}H_8O_7$
2,5,8-Trihydroxy-3-methyl-6,7-methylenedioxy-1,4-naphthoquinone, T-60333

$C_{12}H_8STe$
Phenothiatellurin, P-80086

$C_{12}H_8S_2$
2-Dibenzothiophenethiol, D-60078
4-Dibenzothiophenethiol, D-60079

$C_{12}H_8Se_2$
Selenanthrene, S-80021

$C_{12}H_9BrO$
1-Acetyl-3-bromonaphthalene, A-60021
1-Acetyl-4-bromonaphthalene, A-60022
1-Acetyl-5-bromonaphthalene, A-60023
1-Acetyl-7-bromonaphthalene, A-60024
2-Acetyl-6-bromonaphthalene, A-60025

$C_{12}H_9BrO_3$
2-Bromo-3-ethoxy-1,4-naphthoquinone, *in* B-60268

$C_{12}H_9ClN_2$
3-Chloro-3-(1-naphthylmethyl)diazirine, C-80081

$C_{12}H_9ClO_2S$
[1,1′-Biphenyl]-2-sulfonic acid; Chloride, *in* B-80122
[1,1′-Biphenyl]-3-sulfonic acid; Chloride, *in* B-80123
[1,1′-Biphenyl]-4-sulfonic acid; Chloride, *in* B-80124

$C_{12}H_9IN_2O$
3-Amino-5-iodopyridine; N-Benzoyl, *in* A-80092

$C_{12}H_9IO$
1-Acetyl-7-iodonaphthalene, A-60037
1-Acetyl-8-iodonaphthalene, A-60038

$C_{12}H_9N$
1-Aminobiphenylene, A-80062
2-Aminobiphenylene, A-80063

$C_{12}H_9NO$
Benz[*cd*]indol-2-(1*H*)-one; *N*-Me, *in* B-70027
2-(2-Furanyl)-1*H*-indole, F-80095
3-(2-Furanyl)-1*H*-indole, F-80096
1-Hydroxycarbazole, H-80137
2-Hydroxycarbazole, H-60109
2-Methylfuro[3,2-*c*]quinoline, M-70083

$C_{12}H_9NO_2$
2-Phenyl-3-pyridinecarboxylic acid, P-80125
2-Phenyl-4-pyridinecarboxylic acid, P-80126
4-Phenyl-2-pyridinecarboxylic acid, P-80127
5-Phenyl-2-pyridinecarboxylic acid, P-80128
5-Phenyl-3-pyridinecarboxylic acid, P-80129

$C_{12}H_9N_3$
2-Amino-1,10-phenanthroline, A-70179
4-Amino-1,10-phenanthroline, A-70181
5-Amino-1,10-phenanthroline, A-70182
8-Amino-1,7-phenanthroline, A-70180
2-Phenyl-2*H*-benzotriazole, P-60083
N-Pyridinium-2-benzimidazole, P-70172

$C_{12}H_9N_3O$
3-Amino-β-carboline; N^3-Formyl, *in* A-70110
2-Phenyl-2*H*-benzotriazole; 1-*N*-Oxide, *in* P-60083
Pyridazino[4,5-*b*]quinolin-10(5*H*)-one; 2-Me, *in* P-80207
Pyridazino[4,5-*b*]quinolin-10(5*H*)-one; 5-Me, *in* P-80207

$C_{12}H_{10}$
1,6-Dihydro-1,6-dimethyleneazulene, D-60225
2,6-Dihydro-2,6-dimethyleneazulene, D-60226
1,2-Dihydro-1,2-dimethylenenaphthalene, D-80187
1,2-Dihydro-1,4-dimethylenenaphthalene, D-80188
2,3-Dihydro-2,3-dimethylenenaphthalene, D-80189

$C_{12}H_{10}ClNO$
2-Chloro-1-naphthylamine; *N*-Ac, *in* C-80080

$C_{12}H_{10}F_3NO_2$
7-Amino-4-(trifluoromethyl)-2*H*-1-benzopyran-2-one; *N*-Et, *in* A-60265

$C_{12}H_{10}N_2$
1,5-Diaminobiphenylene, D-80053
2,3-Diaminobiphenylene, D-80054
2,6-Diaminobiphenylene, D-80055
1-(1-Diazoethyl)naphthalene, D-60061
5,6-Dihydrobenzo[*c*]cinnoline, D-80172

$C_{12}H_{10}N_2O$
5-Phenyl-3-pyridinecarboxylic acid; Amide, *in* P-80129

$C_{12}H_{10}N_2OS$
2-(Methylsulfinyl)perimidine, *in* P-10051

$C_{12}H_{10}N_2O_2$
5-Hydroxy-2,2′-bipyridine; Ac, *in* H-80123

$C_{12}H_{10}N_2O_3$
5-Acetyl-2,4(1*H*,3*H*)-pyrimidinedione; 1-Ph, *in* A-60047
3-Nitro-4(1*H*)-pyridone; *N*-Benzyl, *in* N-70063

$C_{12}H_{10}N_2S$
2-(Methylthio)perimidine, *in* P-10051

$C_{12}H_{10}N_4O_2$
[2,2′-Bipyridine]-4,4′-dicarboxylic acid; Diamide, *in* B-60126
[2,2′-Bipyridine]-5,5′-dicarboxylic acid; Diamide, *in* B-60127

$C_{12}H_{10}O$
1,2-Dihydrocyclobuta[*a*]naphthalen-3-ol, D-60215
2,3-Dihydronaphtho[2,3-*b*]furan, D-70235
1-Hydroxyacenaphthene, H-80106
4-Hydroxyacenaphthene, H-60099
3-Methyl-1-naphthaldehyde, M-80120
5-Methyl-1-naphthaldehyde, M-80121
1-Phenyl-2,4-hexadiyn-1-ol, P-80104

$C_{12}H_{10}OS$
5-(Methylthio)-1-phenyl-4-penten-2-yn-1-one, M-80181

$C_{12}H_{10}OS_2$
4-[2,2′-Bithiophen-5-yl]-3-butyn-1-ol, B-80167

$C_{12}H_{10}O_2$
3,4′-Biphenyldiol, B-80106
3-(Hydroxymethyl)-2-naphthalenecarboxaldehyde, H-60188
6-Methoxy-1-naphthaldehyde, *in* H-70184
6-Methoxy-2-naphthaldehyde, *in* H-70185
7-Methoxy-2-naphthaldehyde, *in* H-70186
4-Methyl-1-azulenecarboxylic acid, M-60042
2,3,6,7-Tetrahydro-*as*-indacene-1,8-dione, T-70069
2,3,5,6-Tetrahydro-*s*-indacene-1,7-dione, T-70067
2,3,6,7-Tetrahydro-*s*-indacene-1,5-dione, T-70068

$C_{12}H_{10}O_2S_2$
4-[2,2′-Bithiophen]-5-yl-3-butyne-1,2-diol, B-80166

$C_{12}H_{10}O_3$
2,3,4-Biphenyltriol, B-70124
3,4,5-Biphenyltriol, B-80129

8,8-Dimethyl-1,4,5(8*H*)-naphthalenetrione, D-70421
4-Ethoxy-1,2-naphthoquinone, *in* H-60194
4-Hydroxy-2-cyclopentenone; Benzoyl, *in* H-60116
5-Methoxy-7-methyl-1,2-naphthoquinone, *in* H-60189
8-Methoxy-3-methyl-1,2-naphthoquinone, *in* H-60190
5-Phenyl-2-furancarboxylic acid; Me ester, *in* P-70078

$C_{12}H_{10}O_3S$
[1,1′-Biphenyl]-2-sulfonic acid, B-80122
[1,1′-Biphenyl]-3-sulfonic acid, B-80123
[1,1′-Biphenyl]-4-sulfonic acid, B-80124

$C_{12}H_{10}O_4$
2,2′,3,4-Biphenyltetrol, B-70122
2,2′,3,4-Biphenyltetrol, B-80125
2,3,3′,4-Biphenyltetrol, B-80126
2,3,4,4′-Biphenyltetrol, B-70123
2,3,4,4′-Biphenyltetrol, B-80127
2,3′,4′,5′-Biphenyltetrol, B-80128
5,8-Dihydroxy-2,3-dimethyl-1,4-naphthoquinone, D-60317
3-Hydroxy-5-methoxy-2-methyl-1,4-naphthoquinone, *in* D-60350
6-Hydroxy-5-methoxy-2-methyl-1,4-naphthoquinone, *in* D-60351
1-Oxo-1*H*-2-benzopyran-3-acetic acid; Me ester, *in* O-60058

$C_{12}H_{10}O_5$
Armillarisin A, A-80169
Murraxonin, M-60152

$C_{12}H_{10}O_6S_2$
▷ Benzenesulfonyl peroxide, B-70018

$C_{12}H_{10}O_8$
3,6-Dimethyl-1,2,4,5-benzenetetracarboxylic acid, D-60407
2,5,6,8-Tetrahydroxy-3,7-dimethoxy-1,4-naphthoquinone, *in* H-60065
2,5,7,8-Tetrahydroxy-3,6-dimethoxy-1,4-naphthoquinone, *in* H-60065

$C_{12}H_{10}S$
1,4-Dihydrodibenzothiophene, D-80180
2-(3,5,7-Octatrien-1-ynyl)thiophene, O-80020

$C_{12}H_{11}BrO_3$
5-Bromo-1,2,4-benzenetriol; Tri-Ac, *in* B-70181
6-Bromo-1,2,4-benzenetriol; Tri-Ac, *in* B-70182

$C_{12}H_{11}BrO_6$
2-Bromo-1,3,5-benzenetriol; Tri-Ac, *in* B-60199

$C_{12}H_{11}F_3O_5S$
4,5-Dimethyl-2-phenyl-1,3-dioxol-1-ium; Trifluoromethanesulfonate, *in* D-70431

$C_{12}H_{11}N$
2-(2-Phenylethenyl)-1*H*-pyrrole, P-60094

$C_{12}H_{11}NO$
1,2-Dihydro-3*H*-azepin-3-one; 1-Ph, *in* D-70171
1-Oxo-1,2,3,4-tetrahydrocarbazole, O-70103
2-Oxo-1,2,3,4-tetrahydrocarbazole, O-70104
3-Oxo-1,2,3,4-tetrahydrocarbazole, O-70105
4-Oxo-1,2,3,4-tetrahydrocarbazole, O-70106
4*H*,6*H*-Pyrrolo[1,2-*a*][4,1]benzoxazepine, P-60246

$C_{12}H_{11}NO_2$
1,4-Diacetylindole, *in* A-60033
6-Hydroxy-1-naphthaldehyde; Me ether, oxime, *in* H-70184
6-Hydroxy-2-naphthaldehyde; Me ether, oxime, *in* H-70185

$C_{12}H_{11}NO_2S$
[1,1′-Biphenyl]-3-sulfonic acid; Amide, *in* B-80123
[1,1′-Biphenyl]-4-sulfonic acid; Amide, *in* B-80124

$C_{12}H_{11}NO_3$
3-Amino-1,2-naphthalenediol; *N*-Ac, *in* A-80116
4-Amino-1,2-naphthalenediol; *N*-Ac, *in* A-80117
3-Hydroxy-2-quinolinecarboxylic acid; Me ether, Me ester, *in* H-60228
5-Phenyl-4-oxazolecarboxylic acid; Et ester, *in* P-80112

$C_{12}H_{11}NO_4$
5,6-Dihydroxyindole; *O,O*-Di-Ac, *in* D-70307
1,2-Dimethoxy-4-nitronaphthalene, *in* N-80053
1,4-Dimethoxy-2-nitronaphthalene, *in* N-80050
1,5-Dimethoxy-4-nitronaphthalene, *in* N-80054
2,3-Dimethoxy-6-nitronaphthalene, *in* N-80056
2,6-Dimethoxy-1-nitronaphthalene, *in* N-80048
4,6-Dimethoxy-1-nitronaphthalene, *in* N-80055
2-Oxo-3-indolineglyoxylic acid; Et ester, *in* O-80085

$C_{12}H_{11}N_3$
1,8-Diaminocarbazole, D-80056
Indamine, I-60019
2-(Methylamino)-1*H*-pyrido[2,3-*b*]indole, *in* A-70105

$C_{12}H_{12}$
9,10-Bis(methylene)tricyclo[5.3.0.0^{2,8}]deca-3,5-diene, B-70152
2,3-Didehydro-1,2-dihydro-1,1-dimethylnaphthalene, D-60168
1,4-Dihydrobenzocyclooctatetraene, D-70173
1,6-Dimethylazulene, D-60404
[2.2]Orthometacyclophane, O-80048
Pentacyclo[6.4.0.0^{2,7}.0^{3,12}.0^{6,9}]dodeca-4,10-diene, P-60028
Tetracyclo[6.2.1.1^{3,6}.0^{2,7}]dodeca-2(7),4,9-triene, T-60032
4*a*,4*b*,8*a*,8*b*-Tetrahydrobiphenylene, T-60060
Tricyclo[5.5.0.0^{2,8}]dodeca-3,5,9,11-tetraene, T-80239

$C_{12}H_{12}N_2$
1-Benzyl-5-vinylimidazole, *in* V-70012
2,2′-Diaminobiphenyl, D-60033
4,6-Dimethyl-2-phenylpyrimidine, D-60444
1,4,5,6-Tetrahydrocyclopentapyrazole; 2-Ph, *in* T-80055
4(5)-Vinylimidazole; 1-Benzyl, *in* V-70012

$C_{12}H_{12}N_2O$
5-Amino-1-methylisoquinoline; *N*-Ac, *in* A-80102
1-Oxo-1,2,3,4-tetrahydrocarbazole; (*E*)-Oxime, *in* O-70103
2-Oxo-1,2,3,4-tetrahydrocarbazole; Oxime, *in* O-70104
3-Oxo-1,2,3,4-tetrahydrocarbazole; Oxime, *in* O-70105
4-Oxo-1,2,3,4-tetrahydrocarbazole; Oxime, *in* O-70106
1-Oxo-1,2,3,4-tetrahydrocarbazole; (*Z*)-oxime, *in* O-70103

$C_{12}H_{12}N_2O_2$
2,2′-Dimethoxy-3,3′-bipyridine, *in* D-80287
3,3′-Dimethoxy-2,2′-bipyridine, *in* D-80290
4,4′-Dimethoxy-2,2′-bipyridine, *in* D-80294
5,5′-Dimethoxy-3,3′-bipyridine, *in* D-80298
6,6′-Dimethoxy-2,2′-bipyridine, *in* D-80299
6,6′-Dimethoxy-3,3′-bipyridine, *in* D-80300

$C_{12}H_{12}N_2O_4$
4,4′-Dihydroxy-2,2′-bipyridine; Di-Me ether, 1,1′-dioxide, *in* D-80294

$C_{12}H_{12}N_2O_7$
3-Amino-4-nitro-1,2-benzenedicarboxylic acid; Di-Me ester, Ac, *in* A-70174
4-Amino-3-nitro-1,2-benzenedicarboxylic acid; Di-Me ester, Ac, *in* A-70176
4-Amino-5-nitro-1,2-benzenedicarboxylic acid; Di Me ester, Ac, *in* A-70177

$C_{12}H_{12}N_4O_2$
lin-Benzocaffeine, *in* I-60009
Imidazo[4,5-*g*]quinazoline-6,8(5*H*,7*H*)-dione; 3,5,7-Tri-Me, *in* I-60009

$C_{12}H_{12}N_6$
2,5,8-Trimethylbenzotriimidazole, T-60356

$C_{12}H_{12}N_6O_2$
[2,2′-Bipyridine]-5,5′-dicarboxylic acid; Dihydrazide, *in* B-60127
[3,3′-Bipyridine]-2,2′-dicarboxylic acid; Dihydrazide, *in* B-60133

$C_{12}H_{12}O$
1-Benzoylcyclopentene, B-70072
1-(1-Naphthyl)ethanol, N-70015

$C_{12}H_{12}O_2$
5-Phenyl-2,4-pentadienoic acid; Me ester, *in* P-70086

$C_{12}H_{12}O_2S$
4-Methylthio-2,4-decadiene-6,8-diynoic acid; Me ester, *in* M-80163
5-Methylthio-2,4-decadiene-6,8-diynoic acid; Me ester, *in* M-80164
7-Methylthio-2,6-decadiene-4,8-diynoic acid; Me ester, *in* M-80165
7-Methylthio-2,6-decadiene-4,8-diynoic acid; Me ester, *in* M-80166
7-Methylthio-2,6-decadiene-4,8-diynoic acid; Me ester, *in* M-80166
9-Methylthio-2,8-decadiene-4,6-diynoic acid; Me ester, *in* M-80167
2-(Phenylsulfonyl)-1,3-cyclohexadiene, P-70095

$C_{12}H_{12}O_3$
2,3-Dihydro-3-hydroxy-2-(1-methylethenyl)-5-benzofurancarboxaldehyde, D-70213
4,5-Dimethoxy-1-naphthol, *in* N-60005
4,8-Dimethoxy-1-naphthol, *in* N-60005
4,6-Dimethoxy-5-vinylbenzofuran, *in* D-70352
2,2-Dimethyl-2*H*-1-benzopyran-6-carboxylic acid, D-60408
2-Hydroxycyclopentanone; Benzoyl, *in* H-60114
2-(1-Hydroxy-1-methylethyl)-5-benzofurancarboxaldehyde, *in* D-70214

$C_{12}H_{12}O_3S$
2-Oxo-4-phenylthio-3-butenoic acid; Et ester, *in* O-60088

$C_{12}H_{12}O_3S_3$
2,3,6,7,10,11-Hexahydrobenzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]oxathiin, H-70051

$C_{12}H_{12}O_4$
4,7-Dimethoxy-5-methyl-2*H*-1-benzopyran-2-one, *in* D-60348
4-Hydroxy-2-isopropyl-5-benzofurancarboxylic acid, H-60164

$C_{12}H_{12}O_4S$
7-Methylthio-2,6-decadiene-4,8-diynoic acid; Me ester, S-dioxide, *in* M-80166

$C_{12}H_{12}O_5$
5-Hydroxy-6-(hydroxymethyl)-7-methoxy-2-methyl-4*H*-1-benzopyran-4-one, H-60155
8-(Hydroxymethyl)-5,7-dimethoxy-2*H*-1-benzopyran-2-one, *in* M-80198
Orthosporin, *in* D-80062
5,6,7-Trimethoxy-2*H*-1-benzopyran-2-one, *in* T-80287
5,7,8-Trimethoxy-2*H*-1-benzopyran-2-one, *in* T-80288

$C_{12}H_{12}O_6$
1,4-Benzoquinone-2,6-dicarboxylic acid; Di-Et ester, *in* B-70049
2-Hydroxy-1,4-benzenedicarboxylic acid; Ac, di-Me ester, *in* H-70105

$C_{12}H_{12}S$
1-Methylthio-5-phenyl-1-penten-3-yne, M-80180

$C_{12}H_{12}S_6$
2,3,6,7,10,11-Hexahydrobenzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]dithiin, H-70050

$C_{12}H_{13}BrN_2O_2$
5-Bromotryptophan; Me ester, *in* B-60333

$C_{12}H_{13}N$
1,2,3,4-Tetrahydrocyclopent[*b*]indole; *N*-Me, *in* T-70049

$C_{12}H_{13}NO$
1-Amino-1,4-dihydronaphthalene; *N*-Ac, *in* A-60139
1-Amino-5,8-dihydronaphthalene; *N*-Ac, *in* A-60140
4,5-Dihydro-1,5-ethano-1*H*-1-benzazepin-2(3*H*)-one, D-60239

$C_{12}H_{13}NO_2$
1,4-Dimethoxy-2-naphthylamine, *in* A-80114
2,6-Dimethoxy-1-naphthylamine, *in* A-80112
2,7-Dimethoxy-1-naphthylamine, *in* A-80113
3,4-Dimethoxy-1-naphthylamine, *in* A-80117
3,4-Dimethoxy-2-naphthylamine, *in* A-80116
4,8-Dimethoxy-1-naphthylamine, *in* A-80119
5,6-Dimethoxy-1-naphthylamine, *in* A-80121
5,6-Dimethoxy-2-naphthylamine, *in* A-80124
6,7-Dimethoxy-1-naphthylamine, *in* A-80122
6,7-Dimethoxy-2-naphthylamine, *in* A-80123

$C_{12}H_{13}NO_3$
2,3-Dihydro-2-oxo-1*H*-indole-3-acetic acid; Et ester, *in* D-60259
5,6-Dihydroxyindole; Di-Me ether, *N*-Ac, *in* D-70307
5-Oxo-2-pyrrolidinecarboxylic acid; Benzyl ester, *in* O-70102
1,2,3,4-Tetrahydro-2-oxo-4-quinolinecarboxylic acid; Et ester, *in* T-60077
1,2,3,4-Tetrahydro-4-oxo-7-quinolinecarboxylic acid; Et ester, *in* T-60079

$C_{12}H_{13}NO_7$
2-Hydroxy-5-nitro-1,3-benzenedicarboxylic acid; Di-Et ester, *in* H-70188
4-Hydroxy-3-nitro-1,2-benzenedicarboxylic acid; Di-Et ester, *in* H-70190

$C_{12}H_{13}N_5O_5$
2-Amino-4,7-dihydro-4-oxo-7β-D-ribofuranosyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-5-carbonitrile, A-70132
N^2,3-Ethenoguanosine, *in* I-70006

$C_{12}H_{14}$
Benzylidenecyclopentane, B-70083
1,5,9-Cyclododecatrien-3-yne, C-60190
1,4-Diethynylbicyclo[2.2.2.]octane, D-70157
3,3-Dimethyl-1-phenyl-1-butyne, D-60441
1,3,5,7,9,11-Dodecahexaene, D-70531
as-Hydrindacene, H-60094
s-Hydrindacene, H-60095
[6]-Paracycloph-3-ene, P-70010

$C_{12}H_{14}BrNO_4$
4-(Bromomethyl)-2-nitrobenzoic acid; *tert*-Butyl ester, *in* B-60297

$C_{12}H_{14}N_2$
5-Amino-1-methylisoquinoline; *N*,*N*-Di-Me, *in* A-80102
3-Amino-1,2,3,4-tetrahydrocarbazole, A-60259
1,8-Bis(methylamino)naphthalene, *in* D-70042

$C_{12}H_{14}N_2O_2$
β-Methyltryptophan, M-80187

$C_{12}H_{14}N_2O_3$
1,2,3,4-Tetrahydro-4-oxo-7-quinolinecarboxylic acid; Et ester, oxime, *in* T-60079

$C_{12}H_{14}N_4O_6$
Tetrahydroimidazo[4,5-*d*]imidazole-2,5(1*H*,3*H*)-dione; 1,3,4,6-Tetra-Ac, *in* T-70066

$C_{12}H_{14}O$
2-Acetyl-1,2,3,4-tetrahydronaphthalene, A-70053
Benzoylcyclopentane, B-80055
6-*tert*-Butylcyclopenta[*c*]pyran, B-80284
3,4-Dihydro-2,2-dimethyl-1(2*H*)-naphthalenone, D-60228
3-Methyl-3-phenylcyclopentanone, M-80143
1-Phenyl-5-hexen-1-one, P-70081
6,7,8,9-Tetrahydro-5*H*-benzocycloheptene-6-carboxaldehyde, T-60055
6,7,8,9-Tetrahydro-5*H*-benzocycloheptene-7-carboxaldehyde, T-60056
[5](2,7)Troponophane, T-70330

$C_{12}H_{14}O_2$
3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-carboxaldehyde, D-80185
1,2,3,4,4*a*,10*a*-Hexahydrodibenzo[*b*,*e*][1,4]dioxin, H-80056
Ligustilide, L-60026
1-Phenyl-3-buten-1-ol; Ac, *in* P-70061
4-Phenyl-3-buten-1-ol; Ac, *in* P-80097
Spiro[1,3-benzodioxole-2,1′-cyclohexane], S-80041

$C_{12}H_{14}O_2S$
5-Methylthio-2*Z*,4*E*,6*Z*-decatetrien-8-ynoic acid methyl ester, *in* M-80164
5-Methylthio-2,4,8-decatrien-6-ynoic acid; Me ester, *in* M-80168
3-[(4-Methylthio)phenyl]-2-butenoic acid; Me ester, *in* M-80179
2-[2-(Methylthio)propenyl]benzoic acid; Me ester, *in* M-80182

$C_{12}H_{14}O_3$
3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-carboxylic acid, D-80186
2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-5-benzofurancarboxaldehyde, D-70214
5-Hexynoic acid; Anhydride, *in* H-80086
3-(4-Hydroxyphenyl)-2-propenoic acid; Me ether, Et ester, *in* H-80242
Senkyunolide *F*, *in* L-60026
1,2,3,4-Tetrahydro-1-hydroxy-2-naphthalenecarboxylic acid; Me ester, *in* T-70063

$C_{12}H_{14}O_3S$
2-Mercapto-3-methylbutanoic acid; *S*-Benzoyl, *in* M-60023

$C_{12}H_{14}O_4$
Calaminthone, C-70006
2-(1,2-Dihydroxy-1-methylethyl)-2,3-dihydro-5-benzofurancarboxaldehyde, *in* D-70214
1-(2-Hydroxy-4,6-dimethoxyphenyl)-2-buten-1-one, *in* T-80331
4-Hydroxy-3-(2-hydroxy-3-methyl-3-butenyl)benzoic acid, H-60154
5-(3,4-Methylenedioxyphenyl)pentanoic acid, M-80085
Thurfyl salicylate, *in* H-70108
3-(2,4,5-Trimethoxyphenyl)-2-propenal, T-70278

$C_{12}H_{14}O_5$
2-Hydroxy-1,3-benzenedicarboxylic acid; Di-Et ester, *in* H-60101
5-Hydroxy-3-methyl-1,2-benzenedicarboxylic acid; Me ether, di-Me ester, *in* H-70162
2′,4′,6′-Trihydroxyacetophenone; 2′,4′-Di-Me ether, Ac, *in* T-70248

$C_{12}H_{14}O_6$
4,5-Dihydroxy-1,3-benzenedicarboxylic acid; Di-Me ether, di-Me ester, *in* D-60307

$C_{12}H_{15}^{\oplus}$
Tricyclopropylcyclopropenium(1+), T-60270

$C_{12}H_{15}BF_4$
Tricyclopropylcyclopropenium(1+); Tetrafluoroborate, *in* T-60270

$C_{12}H_{15}BrN_2O_5$
5-(2-Bromovinyl)-2′-deoxyuridine; 3-Me, *in* B-80266
5-(2-Bromovinyl)-2′-deoxyuridine; 3′-Me ether, *in* B-80266

$C_{12}H_{15}BrO_2$
2-Bromo-4-phenylbutanoic acid; Et ester, *in* B-80242

$C_{12}H_{15}Cl$
Tricyclopropylcyclopropenium(1+); Chloride, *in* T-60270

$C_{12}H_{15}F_6Sb$
Tricyclopropylcyclopropenium(1+); Hexafluoroantimonate, *in* T-60270

$C_{12}H_{15}N$
1,2,3,5,10,10*a*-Hexahydropyrrolo[1,2-*b*]isoquinoline, H-70072
Isoindole; *N*-*tert*-Butyl, *in* I-80063
▷ 1,2,3,6-Tetrahydro-1-methyl-4-phenylpyridine, *in* T-60081

$C_{12}H_{15}NO$
Benzoylcyclopentane; Oxime, *in* B-80055

$C_{12}H_{15}NO_2$
2-Amino-3-methyl-3-butenoic acid; Benzyl ester, *in* A-60218
1,2,3,4-Tetrahydro-1-isoquinolinecarboxylic acid; Et ester, *in* T-60070

$C_{12}H_{15}NO_3$
2-Amino-2-methyl-3-phenylpropanoic acid; *N*-Ac, *in* A-60225
2′,3′,4′,5′-Tetramethyl-6′-nitroacetophenone, T-60145
2′,3′,4′,6′-Tetramethyl-5′-nitroacetophenone, T-60146
2′,3′,5′,6′-Tetramethyl-4′-nitroacetophenone, T-60147

$C_{12}H_{15}N_3O_3$
3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]oxazine, H-80054

$C_{12}H_{15}N_3S_3$
3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]thiazine, H-80055

$C_{12}H_{15}N_5O_3$
Queuine, Q-70004

$C_{12}H_{16}$
1,4,7,10-Cyclododecatetraene, C-70217
Pentacyclo[6.3.1.0^{2,4}.0^{5,10}.0^{7,8}]dodecane, P-70019
Tetracyclo[6.2.1.1^{3,6}.0^{2,7}]dodec-2(7)-ene, T-70021
Tetracyclo[6.4.0.0^{4,12}.0^{5,9}]dodec-10-ene, T-70020

$C_{12}H_{16}BrClO$
Furocaespitane, F-60090

$C_{12}H_{16}BrClO_2$
5-(3-Bromo-4-chloro-4-methylcyclohexyl)-5-methyl-2(5*H*)-furanone, B-60222

$C_{12}H_{16}N_2$
1,3-Bis(dimethylamino)pentalene, B-80147
Octahydropyrrolo[3,4-*c*]pyrrole; *N*-Ph, *in* O-70017

$C_{12}H_{16}N_2O_3$
3-[1-(1,1-Dimethyl-3-oxobutyl)imidazol-4-yl]-2-propenoic acid, *in* U-70005

$C_{12}H_{16}N_2O_4$
N-Tyrosylalanine, T-60411

$C_{12}H_{16}N_6O_4$
N^6-(Carbamoylmethyl)-2′-deoxyadenosine, C-70016

$C_{12}H_{16}O$
(1-Adamantyloxy)ethyne, *in* E-80070
4-(4-Methylphenyl)-2-pentanone, M-60112
Pentamethylbenzaldehyde, P-80057

$C_{12}H_{16}O_2$
1,1′-Bi(bicyclo[1.1.1]pentane)-3-carboxylic acid; Me ester, *in* B-80072
4-Isopropylbenzyl alcohol; Ac, *in* I-80078
2-(4-Methylphenyl)propanoic acid; Et ester, *in* M-60114
Tricyclo[4.4.2.0^{1,6}]dodecane-2,7-dione, T-60261
Tricyclo[6.2.1.1^{3,6}]dodecane-2,7-dione, T-80238

$C_{12}H_{16}O_2Se$
4,7-Dihydro-1,1,3,3-tetramethyl-1*H*,3*H*-3*a*,7*a*-episeleno-4,7-epoxyisobenzofuran, D-70266

$C_{12}H_{16}O_3$
Jasmine ketolactone, J-80005
1,2,3,4,5,6,7,8-Octahydro-8-oxo-2-naphthalenecarboxylic acid; Me ester, *in* O-80015
3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid; (Z)-*form*, *in* O-80090
1,2,4-Trimethoxy-5-(2-propenyl)benzene, T-70279
Xanthostemone, X-70002

$C_{12}H_{16}O_4$
6-Ethyl-2,4-dihydroxy-3-methylbenzoic acid; Et ester, *in* E-70041
Senkyunolide *H*, *in* L-60026
Sordariol, S-70056

$C_{12}H_{16}O_5$
3,4,5-Trihydroxyphenylacetic acid; *tert*-Butyl ester, *in* T-60343
2,3,4-Trihydroxyphenylacetic acid; Tri-Me ether, Me ester, *in* T-60340
2,4,5-Trihydroxyphenylacetic acid; Tri-Me ether, Me ester, *in* T-60342

$C_{12}H_{16}O_6$
Diethyl diacetylfumarate, *in* D-80042
Pentamethoxybenzaldehyde, *in* P-60042

$C_{12}H_{16}O_7$
Arbutin, A-70248
Pentamethoxybenzoic acid, *in* P-60043

$C_{12}H_{17}N$
1,2-Dimethyl-5-phenylpyrrolidine, *in* M-80147
[7](2,6)Pyridinophane, P-80212

$C_{12}H_{17}NO$
[7](2,6)Pyridinophane; N-Oxide, *in* P-80212

$C_{12}H_{17}NO_2$
2-Amino-2-methyl-3-phenylpropanoic acid; Et ester, *in* A-60225
Pentamethyl(nitromethyl)benzene, P-80059

$C_{12}H_{17}NO_3$
2-Amino-3-(4-methoxyphenyl)-3-methylbutanoic acid, *in* A-60198

$C_{12}H_{17}NO_5$
3-Hydroxy-1*H*-pyrrole-2,4-dicarboxylic acid; *N*-Me, Me ether, Di-Et ester, *in* H-80251

$C_{12}H_{17}NO_7$
Epivolkenin, *in* T-60007
Innovanamine, *in* H-80214
Taraktophyllin, T-60007

$C_{12}H_{17}N_3O_4$
▷ Agaritine, A-70071

$C_{12}H_{17}N_5O_5$
8-(Dimethylamino)inosine, *in* A-70198

$C_{12}H_{17}N_5O_{10}S$
Antibiotic PB 5266*C*, A-70227

$C_{12}H_{18}$
2*a*,3,4,5,5*a*,6,7,8,8*a*,8*b*-Decahydroacenaphthene, D-80009
2-Isopropyl-1,3,5-trimethylbenzene, I-60130

$C_{12}H_{18}N_2$
1,4-Dihydropyrrolo[3,2-*b*]pyrrole; 1,4-Diisopropyl, *in* D-30286

$C_{12}H_{18}N_4O_4$
Octahydroimidazo[4,5-*d*]imidazole; 1,3,4,6-Tetra-Ac, *in* O-70015

$C_{12}H_{18}N_6O_5$
8-(Dimethylamino)guanosine, *in* A-70150

$C_{12}H_{18}O$
Methoxypentamethylbenzene, *in* P-60058
Pentamethylbenzyl alcohol, P-80058

$C_{12}H_{18}OS$
(Phenylthio)acetaldehyde; Di-Et acetal, *in* P-80136

$C_{12}H_{18}O_2$
Anastrephin, A-70206
[1,1′-Bicyclohexyl]-2,2′-dione, B-60089
Clavularin *A*, C-60153
Clavularin *B*, *in* C-60153
Epianastrephin, *in* A-70206
6-(1-Heptenyl)-5,6-dihydro-2*H*-pyran-2-one, H-60025
1-Hydroxy-11,12,13-trisnor-9-eremophilen-8-one, H-80263
5-Isopropyl-2-methyl-1,3-benzenediol; Di-Me ether, *in* I-60125
Myrtenol; Ac, *in* M-80205
Suspensolide, S-70084

$C_{12}H_{18}O_3$
1*R*-Acetoxy-3-myodesertene, *in* M-80203
1*S*-Acetoxy-3-myodesertene, *in* M-80203
2,10-Dihydroxy-11,12,13-trisnor-6-eremophilen-8-one, D-80391
7-Isojasmonic acid, *in* J-60002
Jasmonic acid, J-60002
Libanotic acid, L-80025
Sedanonic acid, S-80020

$C_{12}H_{18}O_4$
1-Acetoxy-7-hydroxy-3,7-dimethyl-2*E*,5*E*-octadien-4-one, *in* D-60318
3,4-Dihydroxyphenylacetaldehyde; Di-Me ether, di-Me acetal, *in* D-60371

$C_{12}H_{18}O_5$
1-Acetoxy-7-hydroperoxy-3,7-dimethyl-2*E*,5*E*-octadien-4-one, *in* D-60318

$C_{12}H_{18}O_9$
s-Trioxane-2,4,6-tripropionic acid, *in* O-80068

$C_{12}H_{19}N$
3-Azatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane; *N*-Me, *in* A-70282
1,2,3,4,5,6,7,8,8*a*,9*a*-Decahydrocarbazole, D-70012

$C_{12}H_{19}NO_4$
▷ Choline salicylate, *in* H-70108

$C_{12}H_{20}$
1-*tert*-Butyl-1,2-cyclooctadiene, B-60344
Cyclododecyne, C-60192
1,1′,2,2′,3,4,5,5′,6,6′-Decahydrobiphenyl, D-60007
1,1′,2,3,4,4′,5,5′,6,6′-Decahydrobiphenyl, D-60008
1,2,3,3′,4,4′,5,5′,6,6′-Decahydrobiphenyl, D-60009
1,3-Dimethyladamantane, D-70366
5-Dodecen-7-yne, D-70538
Tricyclo[5.5.0.0^{2,8}]dodecane, T-80237

$C_{12}H_{20}BrClO$
Kumepaloxane, K-80013

$C_{12}H_{20}N_2$
7,7′-Bi-7-azabicyclo[2.2.1]heptane, B-80068

$C_{12}H_{20}N_2O_7$
2′-Deoxymugeneic acid, *in* M-60148

$C_{12}H_{20}N_2O_8$
Isomugeneic acid, *in* M-60148
Mugineic acid, M-60148

$C_{12}H_{20}N_2O_9$
3-Hydroxymugeneic acid, *in* M-60148

$C_{12}H_{20}N_4O_4$
Octahydro-1,2,5,6-tetrazocine; Tetra-Ac; *in* O-60020

$C_{12}H_{20}O_2$
10-Dodecen-12-olide, *in* H-60126

$C_{12}H_{20}O_3$
8-Acetoxy-2,6-dimethyl-3,6-octadien-2-ol, *in* D-80457
Cucurbic acid, C-50302
6-Epi-7-isocucurbic acid, *in* C-50302
Helicascolide A, H-80004
Helicascolide B, *in* H-80004
3-Oxo-2-pentylcyclopentaneacetic acid, O-80091

$C_{12}H_{20}O_3S_2$
Asadisulphide, A-80175

$C_{12}H_{20}O_4$
9,12-Dioxododecanoic acid, D-60471
4-Octene-1,8-diol; Di-Ac, *in* O-70026

$C_{12}H_{20}O_6$
1,2-*O*-Cyclohexylidene-*myo*-inositol, *in* I-80015
1,2:4,5-Di-*O*-isopropylidene-*myo*-inositol, *in* I-80015

$C_{12}H_{20}O_8$
Parasorboside, *in* T-60067

$C_{12}H_{20}S$
2,4-Di-*tert*-butylthiophene, D-80112

$C_{12}H_{21}N$
Dodecahydrocarbazole, D-70532

$C_{12}H_{21}NO_4$
2-Amino-1,4-cyclohexanedicarboxylic acid; Di-Et ester, *in* A-60118
3-Amino-1,2-cyclohexanedicarboxylic acid; Di-Et ester, *in* A-60119
4-Amino-1,1-cyclohexanedicarboxylic acid; Di-Et ester, *in* A-60120
4-Amino-1,3-cyclohexanedicarboxylic acid; Di-Et ester, *in* A-60121
3,4-Dihydroxy-2,5-pyrrolidinedione; Di-*tert*-butyl ether, *in* D-80377

$C_{12}H_{21}N_3$
3,5,12-Triazatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane; 3,5,12-Tri-Me, *in* T-70206

$C_{12}H_{22}$
2,3-Di-*tert*-butyl-1,3-butadiene, D-80108

$C_{12}H_{22}Cl_2O$
12-Chlorododecanoic acid; Chloride, *in* C-70066

$C_{12}H_{22}N_2$
1-*tert*-Butyl-3-(*tert*-butylamino)-1*H*-pyrrole, *in* A-80143
1,1-Di-1-piperidinylethene, D-70500

$C_{12}H_{22}N_2O_2$
3,6-Bis(1-methylpropyl)-2,5-piperazinedione, B-70153
3,6-Bis(2-methylpropyl)-2,5-piperazinedione, B-60171
Dihydro-4,6-(1*H*,5*H*)-pyrimidinedione; Di-*tert*-butyl ether, *in* D-70256

$C_{12}H_{22}O$
2,3-Dodecadien-1-ol, D-80520
11-Dodecyn-1-ol, D-70540
5-Dodecyn-1-ol, D-70539
10-Methoxy-1-undecyne, *in* U-80032

$C_{12}H_{22}O_2$
11-Decanolide, *in* H-80157
5-Decen-1-ol; Ac, *in* D-70019
2,6-Dodecanedione, D-70534
Invictolide, I-60038
2-Oxodecanal, O-70087

$C_{12}H_{22}O_2S_2$
2,2,3,3-Tetramethyl-1,4-butanedithiol; Di-Ac, *in* T-80142

$C_{12}H_{22}O_3$
10-Hydroxy-11-dodecenoic acid, H-60125
12-Hydroxy-10-dodecenoic acid, H-60126
12-Oxododecanoic acid, O-60066

$C_{12}H_{22}O_4$
(1-Methylpropyl)butanedioic acid; Di-Et ester, *in* M-80150
Talaromycin *A*, T-70004
Talaromycin *B*, *in* T-70004
Talaromycin *C*, *in* T-70004
Talaromycin *D*, *in* T-70004
Talaromycin *E*, *in* T-70004
Talaromycin *F*, *in* T-70004
Talaromycin *G*, *in* T-70004
1,1,4,4-Tetraethoxy-2-butyne, *in* B-60351
L-Threaric acid; Di-*tert*-butyl ester, *in* T-70005
L-Threaric acid; Di-*tert*-butyl ether, *in* T-70005

$C_{12}H_{22}O_6$
Diethyl diethoxymethylmalonate, *in* H-80204

$C_{12}H_{23}Br$
6-Bromo-6-dodecene, B-60238

$C_{12}H_{23}ClO_2$
12-Chlorododecanoic acid, C-70066

$C_{12}H_{23}NO_2$
1,1′-Iminobis[3,3-dimethyl-2-butanone], I-80008

$C_{12}H_{23}NO_{10}S_2$
Glucocleomin, G-80021

$C_{12}H_{24}$
1,1,2,2,3,3-Hexamethylcyclohexane, H-60070
2,2,3,4,5,5-Hexamethyl-3-hexene, H-70083

$C_{12}H_{24}I_2$
1,12-Diiodododecane, D-80405

$C_{12}H_{24}N_2O_4$
1,12-Dinitrododecane, D-80495

$C_{12}H_{24}N_2O_4S$
Homopantetheine, H-60090

$C_{12}H_{24}O$
9-Dodecen-1-ol, D-70537
2,5,7,7-Tetramethyloctanal, T-70139

$C_{12}H_{24}O_2$
1,1-Dimethoxy-3-decene, *in* D-70016
10-Methylundecanoic acid, M-80188

$C_{12}H_{24}O_3$
11-Hydroxydodecanoic acid, H-80157
7-Hydroxydodecanoic acid, H-80156

$C_{12}H_{24}O_4$
1,1,8,8-Tetramethoxy-4-octene, *in* O-70025

$C_{12}H_{24}S_6$
1,4,7,10,13,16-Hexathiacyclooctadecane, H-70087

$C_{12}H_{26}N_2$
Hexahydropyrimidine; 1,3-Di-*tert*-butyl, *in* H-60056

$C_{12}H_{26}N_2O_4$
1,7,10,16-Tetraoxa-4,13-diazacyclooctadecane, T-60161

$C_{12}H_{26}N_4O_2S_2$
Homoalethine, H-60084

$C_{12}H_{27}NO_6$
Tris[(2-hydroxyethoxy)ethyl]amine, T-70323

$C_{12}H_{27}N_3$
Hexahydro-1,3,5-triazine; 1,3,5-Triisopropyl, *in* H-60060

$C_{12}H_{29}N_5$
1,4,7,10,14-Pentaazacycloheptadecane, P-60019
1,4,7,11,14-Pentaazacycloheptadecane, P-60020

$C_{12}H_{31}N_5$
1,5,9,13,17-Pentaazaheptadecane, P-60026

$C_{13}Cl_9$
Nonachlorophenalenyl, N-60055

$C_{13}H_2F_{10}$
Bis(pentafluorophenyl)methane, B-80158

$C_{13}H_4F_4O$
2,4,5,7-Tetrafluoro-9*H*-fluoren-9-one, T-80052

$C_{13}H_5BrF_{12}O_2$
4-Methyl-2,2,6,6-tetrakis(trifluoromethyl)-2*H*,6*H*-[1,2]bromoxolo[4,5,1-*hi*][1,2]benzobromoxole, M-60128

$C_{13}H_5F_{14}IO_2$
8,8-Difluoro-8,8-dihydro-4-methyl-2,2,6,6-tetrakis(trifluoromethyl)-2*H*,6*H*-[1,2]iodoxolo[4,5,1-*hi*][1,2]benziodoxole, D-60182

$C_{13}H_6Cl_2O_2$
1,5-Dichloroxanthone, D-70139
1,7-Dichloroxanthone, D-70140
2,6-Dichloroxanthone, D-70141
2,7-Dichloroxanthone, D-70142
3,6-Dichloroxanthone, D-70143

$C_{13}H_7ClN_2O_2$
2-Chloro-1-phenazinecarboxylic acid, C-80093
3-Chloro-1-phenazinecarboxylic acid, C-80094
6-Chloro-1-phenazinecarboxylic acid, C-80095
7-Chloro-1-phenazinecarboxylic acid, C-80096
8-Chloro-1-phenazinecarboxylic acid, C-80097
9-Chloro-1-phenazinecarboxylic acid, C-80098

$C_{13}H_7ClO$
2-Biphenylenecarboxylic acid; Chloride, *in* B-80110

$C_{13}H_7FO$
1-Fluoro-9*H*-fluoren-9-one, F-80039
2-Fluoro-9*H*-fluoren-9-one, F-80040
3-Fluoro-9*H*-fluoren-9-one, F-80041
4-Fluoro-9*H*-fluoren-9-one, F-80042

$C_{13}H_7IO$
1-Iodo-9*H*-fluoren-9-one, I-80027
2-Iodo-9*H*-fluoren-9-one, I-80028
3-Iodo-9*H*-fluoren-9-one, I-80029
4-Iodo-9*H*-fluoren-9-one, I-80030

$C_{13}H_7N$
1-Cyanobiphenylene, *in* B-80109
2-Cyanobiphenylene, *in* B-80110

$C_{13}H_7NO_2$
Benzo[*g*]quinoline-6,9-dione, B-60045
Benzo[*h*]quinoline-7,8-dione, B-80039

$C_{13}H_7NS_2$
Thieno[2′,3′:4,5]thieno[2,3-*c*]quinoline, T-80176

$C_{13}H_8$
1,11-Tridecadiene-3,5,7,9-tetrayne, T-80250
1,12-Tridecadiene-3,5,7,9-tetrayne, T-80251
1,3-Tridecadiene-5,7,9,11-tetrayne, T-80252

$C_{13}H_8BrN$
3-Bromo-4-cyanobiphenyl, *in* B-60211

$C_{13}H_8ClNO_2$
2-Chloro-3-nitro-9*H*-fluorene, C-70132

$C_{13}H_8FNO_4$
5-Fluoro-2-nitrophenol; *O*-Benzoyl, *in* F-60061

$C_{13}H_8N_2$
Benz[*f*]imidazo[5,1,2-*cd*]indolizine, B-70021
9-Diazo-9*H*-fluorene, D-60062

$C_{13}H_8N_2O$
Pyrido[3′,4′:4,5]furo[3,2-*b*]indole, P-70174

$C_{13}H_8N_2O_2S$
9-Diazo-9*H*-thioxanthene; 10,10-Dioxide, *in* D-70065

$C_{13}H_8N_2S$
2-Cyano-10*H*-phenothiazine, *in* P-70056
▷ 3-Cyano-10*H*-phenothiazine, *in* P-70057
9-Diazo-9*H*-thioxanthene, D-70065
6*H*-Pyrido[3′,4′:4,5]thieno[2,3-*b*]indole, P-70177

$C_{13}H_8O$
1-Biphenylenecarboxaldehyde, B-80107
2-Biphenylenecarboxaldehyde, B-80108
7-Phenyl-2,4,6-heptatriyn-1-ol, P-80101
7-Phenyl-2-heptene-4,6-diynal, P-80103
2,12-Tridecadiene-4,6,8,10-tetrayn-1-ol, T-80253
2-(1-Undecen-3,5,7,9-tetraynyl)oxirane, *in* T-80252

$C_{13}H_8OS$
5-[5-(3-Buten-1-ynyl)-2-thienyl]-2-penten-4-ynal, *in* B-80281
6*H*-Dibenzo[*b*,*d*]thiopyran-6-one, D-70080
2-(3,4-Epoxy-1-butynyl)-5-(1,3-pentadiynyl)thiophene, E-80015

$C_{13}H_8O_2$
1-Biphenylenecarboxylic acid, B-80109
2-Biphenylenecarboxylic acid, B-80110
2*H*-Naphtho[1,2-*b*]pyran-2-one, N-70011
4*H*-Naphtho[1,2-*b*]pyran-4-one, N-60010
3,5,7,9,11-Tridecapentayne-1,2-diol, T-80259

$C_{13}H_8O_3$
2-(2-Furanyl)-4*H*-1-benzopyran-4-one, F-60084
2-(3-Furanyl)-4*H*-1-benzopyran-4-one, F-60085
Naphtho[1,8-*bc*]pyran-2-carboxylic acid, N-70010
2*H*-Naphtho-[2,3-*b*]pyran-5,10-dione, N-80007
1*H*-Naphtho[2,3-*c*]pyran-5,10-dione, N-80008

$C_{13}H_8O_4$
2,2-Dihydroxy-1*H*-benz[*f*]indene-1,3(2*H*)dione, D-60308
1,2-Dihydroxyxanthone, D-70353
2,4,5-Trihydroxy-9*H*-fluoren-9-one, T-70261

$C_{13}H_8O_5$
2,3,4,5-Tetrahydroxy-9*H*-fluoren-9-one, T-70109
1,3,7-Trihydroxyxanthone, T-80347
1,5,6-Trihydroxyxanthone, T-60349

$C_{13}H_8O_6$
1,2,3,4-Tetrahydroxyxanthone, T-60126
1,2,4,5-Tetrahydroxyxanthone, T-70122
1,3,5,8-Tetrahydroxyxanthone, T-70123
1,3,6,8-Tetrahydroxyxanthone, T-60127
2,3,4,7-Tetrahydroxyxanthone, T-60128

$C_{13}H_8O_7$
1,2,3,4,8-Pentahydroxyxanthone, P-60051
1,2,3,6,8-Pentahydroxyxanthone, P-70036

$C_{13}H_8S$
2-(3-Buten-1-ynyl)-5-(1,3-pentadiynyl)thiophene, B-80280

$C_{13}H_8S_2$
1,6-Tridecadiene-3,9,11-triyne-5,8-dithione, T-80255
5,12-Tridecadiene-2,8,10-triyne-4,7-dithione, T-80256

$C_{13}H_8Se$
9*H*-Fluorene-9-selenone, F-60018

$C_{13}H_9BF_4OS$
2-Phenyl-1,3-benzoxathiol-1-ium; Tetrafluoroborate, *in* P-60084

$C_{13}H_9BrO_2$
3-Bromo[1,1′-biphenyl]-4-carboxylic acid, B-60211

$C_{13}H_9ClN_2O_3$
Indisocin, I-60028

$C_{13}H_9ClO$
5-Chloro-5,6-dihydro-2-(2,4,6-octatriynylidene)-2*H*-pyran, C-80051

$C_{13}H_9ClOS$
2-Chloro-4-[5-(1,3-pentadiynyl)-2-thienyl]-3-butyn-1-ol, *in* P-80025

$C_{13}H_9ClO_2$
5-Chloro-2-(2,4,6-octatriynylidene)-3,7-dioxabicyclo[4.1.0]heptane, *in* C-80051

$C_{13}H_9ClO_4S$
Dibenzo[*b*,*d*]thiopyrylium(1+); Perchlorate, *in* D-70081
Thioxanthylium(1+); Perchlorate, *in* T-70186

$C_{13}H_9ClO_5$
Xanthylium(1+); Perchlorate, *in* X-70003

$C_{13}H_9ClO_5S$
2-Phenyl-1,3-benzoxathiol-1-ium; Perchlorate, *in* P-60084

$C_{13}H_9F$
1-Fluoro-9*H*-fluorene, F-80034
2-Fluoro-9*H*-fluorene, F-80035
3-Fluoro-9*H*-fluorene, F-80036
4-Fluoro-9*H*-fluorene, F-80037
9-Fluoro-9*H*-fluorene, F-80038

$C_{13}H_9F_3O_3S$
3-(Trifluoromethyl)benzenesulfonic acid; Ph ester, *in* T-60283

$C_{13}H_9I$
1-Iodo-9*H*-fluorene, I-80024
2-Iodo-9*H*-fluorene, I-80025
9-Iodo-9*H*-fluorene, I-80026

$C_{13}H_9N$
1-Cyanoacenaphthene, *in* A-70014
2-Cyano-1,2-dihydrocyclobuta[*a*]naphthalene, *in* D-70177

$C_{13}H_9NO$
4-Phenoxybenzonitrile, *in* P-80088
2-Phenylfuro[2,3-*b*]pyridine, P-60104
2-Phenylfuro[3,2-*c*]pyridine, P-60105

$C_{13}H_9NO_2$
1*H*-Benz[*e*]indole-1,2(3*H*)-dione; *N*-Me, *in* B-70026
Benz[*cd*]indol-2-(1*H*)-one; *N*-Ac, *in* B-70027

$C_{13}H_9NO_2S$
10*H*-Phenothiazine-1-carboxylic acid, P-70055
10*H*-Phenothiazine-2-carboxylic acid, P-70056
10*H*-Phenothiazine-3-carboxylic acid, P-70057
10*H*-Phenothiazine-4-carboxylic acid, P-70058

$C_{13}H_9NO_3$
2-Methoxy-3*H*-phenoxazin-3-one, *in* H-60206

$C_{13}H_9NO_4$
4-Phenyl-2,6-pyridinedicarboxylic acid, P-80130

$C_{13}H_9NO_4S$
10*H*-Phenothiazine-2-carboxylic acid; 5,5-Dioxide, *in* P-70056

$C_{13}H_9NS$
2-Phenylthieno[2,3-*b*]pyridine, P-60136

$C_{13}H_9NSe$
2-Phenylbenzoselenazole, P-80090

$C_{13}H_9N_3$
4-Phenyl-1,2,3-benzotriazine, P-80093

$C_{13}H_9N_3O$
2-Azidobenzophenone, A-60338
3-Azidobenzophenone, A-60339
4-Azidobenzophenone, A-60340
1*H*-Benzotriazole; *N*-Benzoyl, *in* B-70068
4-Phenyl-1,2,3-benzotriazine; 2-Oxide, *in* P-80093
4-Phenyl-1,2,3-benzotriazine; 3-Oxide, *in* P-80093

$C_{13}H_9O^{\oplus}$
Xanthylium(1+), X-70003

$C_{13}H_9OS^{\oplus}$
2-Phenyl-1,3-benzoxathiol-1-ium, P-60084

$C_{13}H_9S^{\oplus}$
Dibenzo[*b*,*d*]thiopyrylium(1+), D-70081
Thioxanthylium(1+), T-70186

$C_{13}H_{10}BrN$
Benzo[*a*]quinolizinium(1+); Bromide, *in* B-70043

$C_{13}H_{10}ClNO_4$
Benzo[*a*]quinolizinium(1+); Perchlorate, *in* B-70043

$C_{13}H_{10}F_2$
Difluorodiphenylmethane, D-60184

$C_{13}H_{10}N^{\oplus}$
Benzo[*a*]quinolizinium(1+), B-70043

$C_{13}H_{10}N_2OS$
10*H*-Phenothiazine-1-carboxylic acid; Amide, *in* P-70055
10*H*-Phenothiazine-2-carboxylic acid; Amide, *in* P-70056

$C_{13}H_{10}N_2O_2$
Benzophenone nitrimine, *in* D-60482

$C_{13}H_{10}N_2O_4$
[2,2′-Bipyridine]-3,3′-dicarboxylic acid; Mono-Me ester, *in* B-60124

$C_{13}H_{10}N_4$
4-Amino-1,2,3-benzotriazine; 3-Ph, *in* A-60092
4-Anilino-1,2,3-benzotriazine, *in* A-60092

$C_{13}H_{10}O$
1-Acenaphthenecarboxaldehyde, A-70013
2-(1,3-Butadienyl)-3-(1,3,5-heptatrienyl)oxirane, B-80277
9*H*-Fluoren-1-ol, F-80016
4-Methoxyacenaphthylene, *in* H-70100
Ponticaepoxide, P-80170
2,10,12-Tridecatriene-4,6,8-triyn-1-ol, *in* T-80253

$C_{13}H_{10}OS$
5-[5-(3-Buten-1-ynyl)-2-thienyl]-2-penten-4-yn-1-ol, B-80281
2-Mercaptobenzophenone, M-70020
3-Mercaptobenzophenone, M-70021
4-Mercaptobenzophenone, M-70022
4-[5-(1,3-Pentadiynyl)-7-thienyl]-3-butyn-1-ol, P-80025

$C_{13}H_{10}OS_2$
5-(3-Buten-1-ynyl)-5′ hydroxymethyl-2,2′-bithienyl, B-80279

$C_{13}H_{10}OS_3$
2,2′:5′,2″-Terthiophene-5-methanol, T-80011

$C_{13}H_{10}OSe_2$
Benzoyl phenyl diselenide, B-70077

$C_{13}H_{10}O_2$
1-Acenaphthenecarboxylic acid, A-70014
1,2-Dihydrocyclobuta[*a*]naphthalene-2-carboxylic acid, D-70177
1,2-Dihydro-3*H*-naphtho[2,1-*b*]pyran-3-one, D-80231
2,3-Dihydro-1*H*-naphtho[2,1-*b*]pyran-1-one, D-80232
2,3-Dihydro-4*H*-naphtho[1,2-*b*]pyran-4-one, D-80233
2,3-Dihydro-4*H*-naphtho[2,3-*b*]pyran-4-one, D-80234
3,4-Dihydro-2*H*-naphtho[1,2-*b*]pyran-2-one, D-80235
3,4-Dihydro-1*H*-naphtho[1,2-*c*]pyran-3-one, D-80236
3,4-Dihydro-1*H*-naphtho[2,3-*c*]pyran-1-one, D-80237
3-[5-(2,4-Hexadiynyl)-2-furanyl]-2-propenal, H-80046
7-(3-Hydroxyphenyl)-2-heptene-4,6-diyn-1-ol, H-80234
2-Methoxy-1-biphenylenol, *in* B-80116
11-Tridecene-3,5,7,9-tetrayne-1,2-diol, T-80261

$C_{13}H_{10}O_2S$
5-[4-(2-Furanyl)-3-buten-1-ynyl]-2-thiophenemethanol, F-80093
4-[5-(1,3-Pentadiynyl)-2-thienyl]-3-butyne-1,2-diol, *in* P-80025

$C_{13}H_{10}O_2S_2$
5-(2-Thienylethynyl)-2-thiophenemethanol; Ac, *in* T-80180

$C_{13}H_{10}O_3$
2*H*-3,4-Dihydronaphtho[2,3-*b*]pyran-5,10-dione, D-80230
4′-Hydroxy-2-biphenylcarboxylic acid, H-70111
Mycosinol, M-60154
Mycosinol, M-80202
4-Phenoxybenzoic acid, P-80088
11-Tridecene-3,5,7,9-tetrayne-1,2,13-triol, T-80262

$C_{13}H_{10}O_4$
Coriandrin, C-70198
8,9-Epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-en-4-ol, *in* M-80202
2,4,6-Trihydroxybenzophenone, T-80285

$C_{13}H_{10}O_5$
α-Sorigenin, *in* S-80039

$C_{13}H_{10}O_7$
Nepenthone *A*, *in* T-60333

$C_{13}H_{10}O_8$
5,8-Dihydroxy-2,3-dimethoxy-6,7-methylenedioxy-1,4-naphthoquinone, *in* H-60065

$C_{13}H_{10}S$
2-(3-Buten-1-ynyl)-5-(3-penten-1-ynyl)thiophene, *in* B-80280
9*H*-Fluorene-9-thiol, F-80015
1-Methylnaphtho[2,1-*b*]thiophene, M-60096
2-Methylnaphtho[2,1-*b*]thiophene, M-60097
4-Methylnaphtho[2,1-*b*]thiophene, M-60098
5-Methylnaphtho[2,1-*b*]thiophene, M-60099
6-Methylnaphtho[2,1-*b*]thiophene, M-60100
7-Methylnaphtho[2,1-*b*]thiophene, M-60101
8-Methylnaphtho[2,1-*b*]thiophene, M-60102
9-Methylnaphtho[2,1-*b*]thiophene, M-60103
2-Phenyl-5-(1-propynyl)thiophene, P-80123

$C_{13}H_{10}S_2$
5-(3-Buten-1-ynyl)-5′-methyl-2,2′-bithienyl, *in* B-80279
2-Dibenzothiophenethiol; *S*-Me, *in* D-60078
4-Dibenzothiophenethiol; *S*-Me, *in* D-60079
5,10,12-Tridecadiene-2,8-diyne-4,7-thione, T-80248

$C_{13}H_{11}BrO$
4-Bromodiphenylmethanol, B-60236

$C_{13}H_{11}ClO$
4-Chlorodiphenylmethanol, C-60065
1-Chloro-3,11-tridecadiene-5,7,9-triyn-2-ol, C-80116
2-Chloro-3,11-tridecadiene-5,7,9-triyn-1-ol, C-80117

$C_{13}H_{11}I$
2-Iododiphenylmethane, I-60045
4-Iododiphenylmethane, I-60046

$C_{13}H_{11}N$
1,2-Dihydrobenz[*f*]isoquinoline, D-80170
3,4-Dihydrobenz[*g*]isoquinoline, D-80171
Diphenylmethaneimine, D-60482
9-Methyl-9*H*-carbazole, M-60056

$C_{13}H_{11}NO$
1-Acenaphthenecarboxaldehyde; Oxime, *in* A-70013
1,2-Dihydrocyclobuta[*a*]naphthalene-2-carboxylic acid; Amide, *in* D-70177
1-Methoxy-9*H*-carbazole, *in* H-80137
9-Methyl-9*H*-carbazol-2-ol, *in* H-60109

$C_{13}H_{11}NOS$
2-Phenyl-4*H*-3,1,2-benzooxathiazine, P-60080

$C_{13}H_{11}NO_2$
2,3-Dihydro-1*H*-naphtho[2,1-*b*]pyran-1-one; Oxime, *in* D-80232
2,3-Dihydro-4*H*-naphtho[2,3-*b*]pyran-4-one; Oxime, *in* D-80234
Diphenyl imidocarbonate, *in* C-70019
2-Hydroxy-*N*-phenylbenzamide, *in* H-70108
3-Methyl-2-nitrobiphenyl, M-70098
5-Phenyl-3-pyridinecarboxylic acid; Me ester, *in* P-80129

$C_{13}H_{11}NO_3$
2-Amino-3-methyl-1,4-naphthoquinone; Ac, *in* A-70171

$C_{13}H_{11}NO_4$
2,3-Quinolinedicarboxylic acid; Di-Me ester, *in* Q-80002

$C_{13}H_{11}NS$
2,3-Dihydro-2-phenyl-1,2-benzisothiazole, D-60261

$C_{13}H_{11}N_3$
2-Aminomethyl-1,10-phenanthroline, A-60224
1*H*-Benzotriazole; 1-Benzyl, *in* B-70068
▷ 2,9-Diaminoacridine, D-60027
▷ 3,6-Diaminoacridine, D-60028
▷ 3,9-Diaminoacridine, D-60029
1-(Dimethylamino)-γ-carboline, *in* A-70114

$C_{13}H_{11}N_3O$
3-Amino-β-carboline; N^3-Ac, *in* A-70110
1,3-Dihydro-2*H*-imidazo[4,5-*c*]pyridin-2-one; 1-Benzyl, *in* D-60250
Pyridazino[4,5-*b*]quinolin-10(5*H*)-one; 5-Et, *in* P-80207

$C_{13}H_{12}$
Benz[*f*]indane, B-60015
Bicyclo[6.4.1]trideca-1,3,5,7,9,11-hexaene, B-80091
3-Methylbiphenyl, M-60053
Tetracyclo[5.5.1.$0^{4,13}$.$0^{10,13}$]trideca-2,5,8,11-tetraene, T-60036

$C_{13}H_{12}N_2$
N,N'-Diphenylformamidine, D-60479

$C_{13}H_{12}N_2O$
2-(Aminomethyl)pyridine; *N*-Benzoyl, *in* A-60227
4-(Aminomethyl)pyridine; *N*-Benzoyl, *in* A-60229
▷ *N,N'*-Diphenylurea, D-70499

$C_{13}H_{12}N_2O_2$
1-Benzyloxy-2-phenyldiazene 2-oxide, *in* H-70208
2,2'-(1,3-Dioxan-2-ylidene)bispyridine, *in* D-70502

$C_{13}H_{12}N_2O_3S$
Aminoiminomethanesulfonic acid; *N,N*-Di-Ph, *in* A-60210

$C_{13}H_{12}N_2O_4S$
Benzenediazo-*p*-toluenesulfonate *N*-oxide, *in* H-70208

$C_{13}H_{12}N_2Se$
Selenourea; N^1,N^1-Di-Ph, *in* S-70031
Selenourea; N^1,N^3-Di-Ph, *in* S-70031

$C_{13}H_{12}N_4$
4-Amino-1*H*-imidazo[4,5-*c*]pyridine; 4-*N*-Benzyl, *in* A-70161

$C_{13}H_{12}O$
2,5-Dihydro-2-(4,6,8-nonatrien-2-ynylidene)furan, D-80238
4-Methoxyacenaphthene, *in* H-60099
1-(1-Naphthyl)-2-propanone, N-80012
1-(2-Naphthyl)-2-propanone, N-80013
3,5-Tridecadiene-7,9,11-triyn-1-ol, T-80258
2,8,10,12-Tridecatetraene-4,6-diyn-1-ol, T-80260

$C_{13}H_{12}O_2$
2-(Benzyloxy)phenol, B-60072
3-(Benzyloxy)phenol, B-60073
▷ 4-(Benzyloxy)phenol, B-60074
3,4-Epoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]nonane, *in* H-80047
▷ Goniothalamin, G-60031
4-Methyl-1-azulenecarboxylic acid; Me ester, *in* M-60042
3,11-Tridecadiene-5,7,9-triyne-1,2-diol, T-80254

$C_{13}H_{12}O_2S_2$
4-[5'-Methyl[2,2'-bithiophen]-5-yl]-3-butyne-1,2-diol, M-70054

$C_{13}H_{12}O_3$
6-Acetyl-5-hydroxy-2-isopropenylbenzo[*b*]furan, *in* A-60065
Goniothalamin oxide, *in* G-60031
7-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.4]non-8-en-3-ol, H-80047
3,11-Tridecadiene-5,7,9-triyne-1,2,13-triol, T-80257

$C_{13}H_{12}O_3S$
[1,1'-Biphenyl]-2-sulfonic acid; Me ester, *in* B-80122
[1,1'-Biphenyl]-3-sulfonic acid; Me ester, *in* B-80123
[1,1'-Biphenyl]-4-sulfonic acid; Me ester, *in* B-80124

$C_{13}H_{12}O_4$
6-Acetyl-5-hydroxy-2-(1-hydroxymethylvinyl)benzo[*b*]furan, *in* A-60065
Altholactone, A-60083
Dihydrocoriandrin, *in* C-70198
5,8-Dihydroxy-2,3,6-trimethyl-1,4-naphthoquinone, D-60380
5,6-Dimethoxy-2-methyl-1,4-naphthoquinone, *in* D-60351
1,4,5-Naphthalenetriol; 5-Me ether, 1-Ac, *in* N-60005
2-Oxo-2*H*-benzopyran-4-acetic acid; Et ester, *in* O-60057
Platypterophthalide, P-60161

$C_{13}H_{12}O_5$
Acuminatolide, A-70063

$C_{13}H_{12}O_7$
5,8-Dihydroxy-2,3,6-trimethoxy-1,4-benzoquinone, *in* P-70033

$C_{13}H_{12}S$
2-Mercaptodiphenylmethane, M-80024

$C_{13}H_{12}S_2$
5-(1-Propenyl)-5'-vinyl-2,2'-bithienyl, P-80182

$C_{13}H_{13}BrN_2O_3$
5-Bromotryptophan; N^{α}-Ac, *in* B-60333
6-Bromotryptophan; N^{α}-Ac, *in* B-60334
7-Bromotryptophan; N^{α}-Ac, *in* B-60335

$C_{13}H_{13}BrO_2$
2-Bromo-3,4-dihydro-1-naphthalenecarboxaldehyde; Ethylene acetal, *in* B-80198
1-Bromo-(2-dimethoxymethyl)naphthalene, *in* B-60302

$C_{13}H_{13}IO_8$
1,1,1-Triacetoxy-1,1-dihydro-1,2-benziodoxol-3(1*H*)-one, T-60228

$C_{13}H_{13}N$
2-Amino-3-methylbiphenyl, A-70164
N-Methyldiphenylamine, M-70060
2-(2-Phenylethenyl)-1*H*-pyrrole; *N*-Me, *in* P-60094
2-(2-Phenylethenyl)-1*H*-pyrrole; *N*-Me, *in* P-60094
1,2,3,4-Tetrahydrobenz[*g*]isoquinoline, T-80054

$C_{13}H_{13}NO$
1-Oxo-1,2,3,4-tetrahydrocarbazole; *N*-Me, *in* O-70103
1,3,4,10-Tetrahydro-9(2*H*)-acridinone, T-60052

$C_{13}H_{13}NO_2$
3-Hydroxy-2-methyl-4(1*H*)-pyridinone; Benzyl ether, *in* H-80214
5-Methyl-1*H*-pyrrole-2-carboxylic acid; Benzyl ester, *in* M-60124

$C_{13}H_{13}NO_3$
2-Formyl-1*H*-indole-3-acetic acid; Et ester, *in* F-80075

$C_{13}H_{13}NO_4$
5,6-Dihydroxyindole; *N*-Me, di-*O*-Ac, *in* D-70307

$C_{13}H_{13}N_3$
3-Amino-β-carboline; N^3-Et, *in* A-70110

$C_{13}H_{13}N_3O_5$
Antibiotic PDE I, A-60286

$C_{13}H_{14}$
2,3,5,6,7-Pentamethylenebicyclo[2.2.2]octane, P-60056

$C_{13}H_{14}N_2$
1,4,5,6-Tetrahydrocyclopentapyrazole; 2-Benzyl, *in* T-80055

$C_{13}H_{14}N_2O$
1-Oxo-1,2,3,4-tetrahydrocarbazole; *N*-Me, oxime, *in* O-70103

$C_{13}H_{14}N_2O_4S_3$
Gliotoxin *E*, G-60024

$C_{13}H_{14}N_4OS_2$
S,S-Bis(4,6-dimethyl-2-pyrimidinyl)dithiocarbonate, B-70138

$C_{13}H_{14}O$
3-Isopropyl-2-naphthol, I-70095
4-Isopropyl-1-naphthol, I-70096
1-(1-Naphthyl)-2-propanol, N-60015

$C_{13}H_{14}OS$
9-(2-Thienyl)-4,6-nonadien-8-yn-1-ol, T-80181
9-(2-Thienyl)-4,6-nonadien-8-yn-3-ol, *in* T-80181

$C_{13}H_{14}O_2$
2-Methyl-4-phenyl-3-butyn-2-ol; Ac, *in* M-70110
7-Phenyl-5-heptynoic acid, P-60106
3,5,11-Tridecadiene-7,9-diyne-1,2-diol, T-80247

$C_{13}H_{14}O_2S$
2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene, M-80175

$C_{13}H_{14}O_3$
4-Acetyl-2,3-dihydro-5-hydroxy-2-isopropenylbenzofuran, A-70040
5-Acetyl-2-(1-hydroxy-1-methylethyl)benzofuran, A-70044
2,2-Dimethyl-2*H*-1-benzopyran-6-carboxylic acid; Me ester, *in* D-60408
7-Ethoxy-3,4-dimethylcoumarin, *in* H-60119
1,4,5-Trimethoxynaphthalene, *in* N-60005

$C_{13}H_{14}O_3S$
2-[(5-Methylsulfinyl)-4-penten-2-ynylidene]-1,6-dioxaspiro[4.4]non-3-ene, *in* M-80175

$C_{13}H_{14}O_4$
6-Acetyl-5-hydroxy-2-hydroxymethyl-2-methylchromene, A-60031
Anaphatol, *in* D-60339
4-Hydroxy-2-isopropyl-5-benzofurancarboxylic acid; Me ester, *in* H-60164
2-Isopropylidene-4,6-dimethoxy-3(2*H*)-benzofuranone, I-80080
3-Phenyl-1,1-cyclopentanedicarboxylic acid, P-80098

$C_{13}H_{14}O_5$
Caleteucrin, C-80012
Diaporthin, D-80062
Salicifoliol, S-80003

$C_{13}H_{14}O_6$
3,4-Dihydroxybenzyl alcohol; Tri-Ac, *in* D-80284

$C_{13}H_{15}ClO$
2-Phenylcyclohexanecarboxylic acid; Chloride, *in* P-70065

$C_{13}H_{15}Cl_2NO_3$
6-Amino-2,2-dichlorohexanoic acid; *N*-Benzoyl, *in* A-60126

$C_{13}H_{15}NO_2$
1-Oxa-2-azaspiro[2,5]octane; *N*-Benzoyl, *in* O-70052

$C_{13}H_{15}NO_3$
2-Pyrrolidinecarboxaldehyde; *N*-Benzyloxycarbonyl, *in* P-70184

$C_{13}H_{15}N_3$
2,6-Bis(3,4-Dihydro-2*H*-pyrrol-5-yl)pyridine, B-80146

$C_{13}H_{15}N_3O_2$
3-Amino-1*H*-pyrazole-4-carboxylic acid; *N*(1)-Benzyl, Et ester, *in* A-70187

$C_{13}H_{16}Br_2$
2,2-Dibromo-2,3-dihydro-1,1,3,3-tetramethyl-1*H*-indene, D-80089

$C_{13}H_{16}Cl_2O_4$
1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone, D-60129

$C_{13}H_{16}N_2$
1,8-Diaminonaphthalene; *N,N,N'*-Tri-Me, *in* D-70042
2-Diazo-1,1,3,3-tetramethylindane, D-60067

$C_{13}H_{16}N_2O_2$
β-Methyltryptophan; Me ester, *in* M-80187

$C_{13}H_{16}N_2O_4$
Bursatellin, B-60338

$C_{13}H_{16}N_4$
Tetrakis(2-cyanoethyl)methane, *in* M-70036

$C_{13}H_{16}O$
▷ Benzoylcyclohexane, B-70071
1-Phenyl-6-hepten-1-one, P-70080
7-Phenyl-3-heptyn-2-ol, P-60107
1,1,3,3-Tetramethyl-2-indanone, T-60143
8,10-Tridecadiene-4,6-diyn-1-ol, T-80249

$C_{13}H_{16}OS$
9-(2-Thienyl)-6-nonen-8-yn-3-ol, *in* T-80181

$C_{13}H_{16}O_2$
3,4-Dihydro-3,3,8*a*-trimethyl-1,6(2*H*,8*aH*)-naphthalenedione, D-60301
6-(3,4-Methylenedioxylphenyl)-1-hexene, *in* M-50261
5-Oxo-5-phenylpentanal; Di-Me acetal, *in* O-80094
2-Phenylcyclohexanecarboxylic acid, P-70065

$C_{13}H_{16}O_3$
3-Benzoyl-2-methylpropanoic acid; Et ester, *in* B-60064
6,7-Dimethoxy-2,2-dimethyl-2*H*-1-benzopyran, D-70365
1-(Dimethoxymethyl)-2,3,5,6-tetrakis(methylene)-7-oxabicyclo[2.2.1]heptane, D-60399
Flossonol, F-60014
5-(1-Hydroxyethyl)-2-(1-hydroxy-1-methylethyl)benzofuran, *in* A-70044
Methyl 3-(4-methoxy-2-vinylphenyl)propanoate, *in* H-70232
Moskachan B, M-50261

$C_{13}H_{16}O_3S$
2-Mercapto-3-methylpentanoic acid; *S*-Benzoyl, *in* M-80026

$C_{13}H_{16}O_4$
4-Hydroxy-3-(2-hydroxy-3-methyl-3-butenyl)benzoic acid; Me ester, *in* H-60154
1-Phenyl-1,2-propanediol; Di-Ac, *in* P-80121
1-(2,4,6-Trimethoxyphenyl)-2-buten-1-one, *in* T-80331

$C_{13}H_{16}O_5$
Emehetin, E-80012

$C_{13}H_{16}O_7$
2-Oxo-1,3-cyclopentanediglyoxylic acid; Di-Et ester, *in* O-70085

$C_{13}H_{16}O_{10}$
6-Galloylglucose, G-80001

$C_{13}H_{16}Se$
1,1,3,3-Tetramethyl-2-indaneselone, T-60142

$C_{13}H_{17}N$
1,3,4,6,7,11*b*-Hexahydro-2*H*-benzo[*a*]quinolizine, H-80053

$C_{13}H_{17}NO$
Benzoylcyclohexane; (*E*)-Oxime, *in* B-70071

$C_{13}H_{17}NO_3S$
2-Amino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylic acid; Et ester, *N*-Ac, *in* A-60258

$C_{13}H_{17}NO_4$
2-Amino-3-(4-hydroxyphenyl)-3-methylbutanoic acid; *N*-Ac, *in* A-60198

$C_{13}H_{18}$
2-Phenyl-2-heptene, P-80102

$C_{13}H_{18}BrClO_3$
Methyl 3-(3-bromo-4-chloro-4-methylcyclohexyl)-4-oxo-2-pentenoate, M-60054

$C_{13}H_{18}N_2$
Octahydropyrrolo[3,4-*c*]pyrrole; *N*-Benzyl, *in* O-70017
1,1,3,3-Tetramethyl-2-indanone; Hydrazone, *in* T-60143

$C_{13}H_{18}N_4O_3$
Citrulline; α-*N*-Benzoyl, amide, *in* C-60151

$C_{13}H_{18}N_4O_4$
4-Amino-4,6-dihydro-3-methyl-1*H*-cyclopenta[*e*]1,2,4-triazine-5,7-dicarboxylic acid; Di-Et ester, *in* A-80066

$C_{13}H_{18}O$
Tricyclone, T-80242

$C_{13}H_{18}O_2$
Pentamethylphenol; Ac, *in* P-60058
(Pentamethylphenyl)acetic acid, P-70038

$C_{13}H_{18}O_3$
Moskachan C, *in* M-50261
1,2,3,4,5,6,7,8-Octahydro-8-oxo-2-naphthalenecarboxylic acid; Et ester, *in* O-80015

$C_{13}H_{18}O_4$
3,4-Dihydroxybutanoic acid; O^4-Benzyl, Et ester, *in* D-60313
1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene, T-80136

$C_{13}H_{18}O_5$
2,2,8,8-Tetramethyl-3,4,5,6,7-nonanepentone, T-60148

$C_{13}H_{18}O_7$
Isosalicin, I-80090
Methylarbutin, *in* A-70248
Pentahydroxybenzoic acid; Penta-Me ether, Me ester, *in* P-60043

$C_{13}H_{18}O_8$
Calleryanin, *in* D-80284
Idesin, *in* D-80283
Salirepin, *in* D-70287

$C_{13}H_{18}O_9$
MP-10, *in* H-80196

$C_{13}H_{19}N$
[8](2,6)Pyridinophane, P-80213

$C_{13}H_{19}NO$
[8](2,6)Pyridinophane; *N*-Oxide, *in* P-80213

$C_{13}H_{19}NO_4$
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid; Di-Et ester, *in* D-80193

$C_{13}H_{19}N_3$
2,6-Bis(2-pyrrolidinyl)pyridine, B-80160

$C_{13}H_{19}N_5O_{10}S$
Antibiotic PB 5266*A*, A-70225

$C_{13}H_{19}N_5O_{11}S$
Antibiotic PB 5266*B*, A-70226

$C_{13}H_{20}$
2-Isopropylideneadamantane, I-60121
Tetracyclo[5.5.1.$0^{4,13}$.$0^{10,13}$]tridecane, T-60035

$C_{13}H_{20}N_6O_3$
3′-Amino-3′-deoxyadenosine; 3′,6,6-Tri-*N*-Me, *in* A-70128

$C_{13}H_{20}O$
γ-Ionone, I-70058

$C_{13}H_{20}O_2$
Prosopidione, P-80183

$C_{13}H_{20}O_3$
Grasshopper ketone, G-70028
Methyl jasmonate, *in* J-60002

$C_{13}H_{20}O_6$
2,2,8,8-Tetramethyl-5,5-dihydroxy-3,4,6,7-nonanetetrone, *in* T-60148

$C_{13}H_{20}O_8$
Methanetetrapropanoic acid, M-70036

$C_{13}H_{21}N$
1,2,3,4,5,6,7,8,8*a*,9*a*-Decahydrocarbazole; *N*-Me, *in* D-70012

$C_{13}H_{21}NO_6$
2,6-Bis(hydroxyacetyl)pyridine; Bis di-Me ketal, *in* B-70144

$C_{13}H_{22}$
1,1,2,2,4,4-Hexamethyl-3,5-bis(methylene)cyclopentane, H-70082

$C_{13}H_{22}O$
1-Cyclododecenecarboxaldehyde, C-60191
Octahydro-5,5,8*a*-trimethyl-2(1*H*)-naphthalenone, *in* D-70014
Theaspirone, T-60185

$C_{13}H_{22}O_4$
9,12-Dioxododecanoic acid; Me ester, *in* D-60471

$C_{13}H_{22}O_5$
4,4-Pyrandiacetic acid; Di-Et ester, *in* P-70150

$C_{13}H_{24}$
Octamethylcyclopentene, O-60026
6,7-Tridecadiene, T-60272

$C_{13}H_{24}O$
Decahydro-5,5,8*a*-trimethyl-2-naphthalenol, D-70014
Dicyclohexylmethanol, D-70150
Octamethylcyclopentanone, O-60025
1,2,2,3,3,4,4,5-Octamethyl-6-oxabicyclo[3.1.0]hexane, O-70021
3-Tridecyn-1-ol, T-80264
6-Tridecyn-1-ol, T-80265

$C_{13}H_{24}O_2$
9-Dodecen-1-ol; Formyl, *in* D-70537

$C_{13}H_{24}O_3$
10-Hydroxy-11-dodecenoic acid; Me ester, *in* H-60125
12-Hydroxy-10-dodecenoic acid; Me ester, *in* H-60126
7-Megastigmene-5,6,9-triol, M-60012
12-Oxododecanoic acid; Me ester, *in* O-60066

$C_{13}H_{24}O_4$
Hexamethylpentanedioic acid; Di-Me ester, *in* H-80076

$C_{13}H_{25}N_3$
11-Methylene-1,5,9-triazabicyclo[7.3.3]pentadecane, M-60080

$C_{13}H_{26}O$
2,2,3,3,4,4,5,5-Octamethylcyclopentanol, O-60024
6-Tridecen-1-ol, T-80263

$C_{13}H_{26}O_3$
11-Hydroxydodecanoic acid; Me ester, *in* H-80157

$C_{13}H_{26}O_4$
10-Oxodecanoic acid; Me ester, Di-Me acetal, *in* O-60063

$C_{13}H_{27}N$
2,6-Di-*tert*-butylpiperidine, D-80111

$C_{13}H_{31}N_5$
1,4,7,11,15-Pentaazacyclooctadecane, P-60023
1,4,8,11,15-Pentaazacyclooctadecane, P-60024

$C_{14}H_4Cl_2O_4$
2,3-Dichloro-1,4,9,10-anthracenetetrone, D-60117

$C_{14}H_4N_6O_{15}$
2,4,6-Trinitrobenzoic acid; Anhydride, *in* T-70303

$C_{14}H_5ClO_4$
2-Chloro-1,4,9,10-anthracenetetrone, C-60041

$C_{14}H_6Cl_2O_2$
1,5-Biphenylenedicarboxylic acid; Dichloride, *in* B-80111
1,8-Biphenylenedicarboxylic acid; Dichloride, *in* B-80112
2,6-Biphenylenedicarboxylic acid; Dichloride, *in* B-80114
2,7-Biphenylenedicarboxylic acid; Dichloride, *in* B-80115

$C_{14}H_6N_4O_{11}$
3,5-Dinitrobenzoic acid; Anhydride, *in* D-60458

$C_{14}H_6O_8$
▷ Ellagic acid, E-70007

$C_{14}H_8$
2,7-Diethynylnaphthalene, D-70158

$C_{14}H_8Br_2$
Bis(2-bromophenyl)ethyne, B-80140
Bis(4-bromophenyl)ethyne, B-80141
2,3-Dibromoanthracene, D-70085
9,10-Dibromoanthracene, D-60085

$C_{14}H_8ClNO$
9-Acridinecarboxylic acid; Chloride, *in* A-70061

$C_{14}H_8Cl_2$
9,10-Dichloroanthracene, D-60116
1,4-Dichlorophenanthrene, D-70132
2,4-Dichlorophenanthrene, D-70133
3,6-Dichlorophenanthrene, D-70134
3,9-Dichlorophenanthrene, D-70135
4,5-Dichlorophenanthrene, D-70136
9,10-Dichlorophenanthrene, D-70137

$C_{14}H_8Cl_2O_2S$
2,2′-Thiobisbenzoic acid; Dichloride, *in* T-70174
4,4′-Thiobisbenzoic acid; Dichloride, *in* T-70175

$C_{14}H_8F_2$
9,10-Difluoroanthracene, D-70161
4,5-Difluorophenanthrene, D-70166
9,10-Difluorophenanthrene, D-70167

$C_{14}H_8F_2O_4$
4,4′-Difluoro-[1,1′-biphenyl]-3,3′-dicarboxylic acid, D-60178
4,5-Difluoro-[1,1′-biphenyl]-2,3-dicarboxylic acid, D-60179
6,6′-Difluoro-[1,1′-biphenyl]-2,2′-dicarboxylic acid, D-60180

$C_{14}H_8F_6O_5S$
3-(Trifluoromethyl)benzenesulfonic acid; Anhydride, *in* T-60283

$C_{14}H_8FeN_2O_8$
Actinoviridin *A*, *in* H-70193

$C_{14}H_8I_2$
9,10-Diiodoanthracene, D-70355
2,7-Diiodophenanthrene, D-70360
3,6-Diiodophenanthrene, D-70361

$C_{14}H_8N_2$
9-Cyanoacridine, *in* A-70061
5,6-Dicyanoacenaphthene, *in* A-70015
Naphtho[8,1,2-*cde*]cinnoline, N-70007
Pyrido[2′,3′:3,4]cyclobuta[1,2-*g*]quinoline, P-60232
Pyrido[3′,2′:3,4]cyclobuta[1,2-*g*]quinoline, P-60233

$C_{14}H_8N_2O$
Naphtho[8,1,2-*cde*]cinnoline; *N*-Oxide, *in* N-70007

$C_{14}H_8N_2O_2$
[1,4]Benzoxazino[3,2-*b*][1,4]benzoxazine, B-60055
1,10-Phenanthroline-2,9-dicarboxaldehyde, P-80085

$C_{14}H_8N_2S$
[1]Benzothieno[2,3-*c*][1,5]naphthyridine, B-70060
[1]Benzothieno[2,3-*c*][1,7]naphthyridine, B-70061

$C_{14}H_8N_2Se$
Phenanthro[9,10-*c*][1,2,5]selenadiazole, P-70053

$C_{14}H_8N_4S_2$
[1,2,4,5]Tetrazino[3,4-*b*:6,1-*b*′]bisbenzothiazole, T-60171

$C_{14}H_8O$
Acenaphtho[5,4-*b*]furan, A-60014

$C_{14}H_8OS$
Phenanthro[4,5-*bcd*]thiophene; 4-Oxide, *in* P-60077

$C_{14}H_8O_2$
Benz[*a*]azulene-1,4-dione, B-60011
1,8-Biphenylenedicarboxaldehyde, B-60118

$C_{14}H_8O_2S$
Phenanthro[4,5-*bcd*]thiophene; 4,4-Dioxide, *in* P-60077

$C_{14}H_8O_3$
3,4-Acenaphthenedicarboxylic acid; Anhydride, *in* A-60013
4-Oxo-4*H*-naphtho[2,3-*b*]pyran-3-carboxaldehyde, O-80088

$C_{14}H_8O_4$
1,5-Biphenylenedicarboxylic acid, B-80111
1,8-Biphenylenedicarboxylic acid, B-80112
2,3-Biphenylenedicarboxylic acid, B-80113
2,6-Biphenylenedicarboxylic acid, B-80114
2,7-Biphenylenedicarboxylic acid, B-80115

$C_{14}H_8O_5$
8-Hydroxyxanthone-1-carboxylic acid, H-80266

$C_{14}H_8O_9$
Luteolic acid, L-80052

$C_{14}H_8S$
Acenaphtho[1,2-*b*]thiophene, A-70017
Acenaphtho[5,4-*b*]thiophene, A-60015
Phenanthro[4,5-*bcd*]thiophene, P-60077

$C_{14}H_8SSe$
[1]Benzoselenopheno[2,3-*b*][1]benzothiophene, B-70052

$C_{14}H_8S_2$
[1]Benzothiopyrano[6,5,4-*def*][1]benzothiopyran, B-60049

$C_{14}H_8Se_4$
Dibenzotetraselenofulvalene, D-70077

$C_{14}H_9BrO$
10-Bromoanthrone, B-80173

$C_{14}H_9ClN_2$
1-Chloro-4-phenylphthalazine, C-70141
2-Chloro-3-phenylquinoxaline, C-70145
6-Chloro-2-phenylquinoxaline, C-70146
7-Chloro-2-phenylquinoxaline, C-70147

$C_{14}H_9ClN_2O$
2-Chloro-3-phenylquinoxaline; 4-Oxide, *in* C-70145
6-Chloro-2-phenylquinoxaline; 4-Oxide, *in* C-70146
7-Chloro-2-phenylquinoxaline; 4-Oxide, *in* C-70147

$C_{14}H_9ClN_2O_2$
6-Chloro-2-phenylquinoxaline; 1,4-Dioxide (?), *in* C-70146

$C_{14}H_9ClO_2$
2-Benzoylbenzoic acid; Chloride, *in* B-80054

$C_{14}H_9Cl_2NO_2$
2,2′-Iminodibenzoic acid; Dichloride, *in* I-60014

$C_{14}H_9NO$
1-Acridinecarboxaldehyde, A-70056
2-Acridinecarboxaldehyde, A-70057
3-Acridinecarboxaldehyde, A-70058
4-Acridinecarboxaldehyde, A-70059
9-Acridinecarboxaldehyde, A-70060
o-Cyanobenzophenone, *in* B-80054
2-Phenyl-3*H*-indol-3-one, P-60114

$C_{14}H_9NO_2$
9-Acridinecarboxaldehyde; 10-Oxide, *in* A-70060
9-Acridinecarboxylic acid, A-70061
4-Phenyl-2*H*-1,3-benzoxazin-2-one, P-80094
3-(Phenylimino)-1(3*H*)-isobenzofuranone, P-60112
2-Phenylisatogen, *in* P-60114
2-(2-Pyridyl)-1,3-indanedione, P-60241
2-(3-Pyridyl)-1,3-indanedione, P-60242
2-(4-Pyridyl)-1,3-indanedione, P-60243

$C_{14}H_9NO_3$
1-Amino-2-hydroxyanthraquinone, A-60174
▷ 1-Amino-4-hydroxyanthraquinone, A-60175
1-Amino-5-hydroxyanthraquinone, A-60176
1-Amino-8-hydroxyanthraquinone, A-60177
2-Amino-1-hydroxyanthraquinone, A-60178
2-Amino-3-hydroxyanthraquinone, A-60179
3-Amino-1-hydroxyanthraquinone, A-60180
9-Amino-10-hydroxy-1,4-anthraquinone, A-60181
1*H*-Benz[*e*]indole-1,2(3*H*)-dione; *N*-Ac, *in* B-70026

$C_{14}H_9NO_4$
(2-Nitrophenyl)phenylethanedione, N-70058
(4-Nitrophenyl)phenylethanedione, N-70059

$C_{14}H_9NS$
10*H*-[1]Benzothieno[3,2-*b*]indole, B-70059
6*H*-[1]Benzothieno[2,3-*b*]indole, B-70058
Pyrrolo[3,2,1-*kl*]phenothiazine, P-70196

$C_{14}H_9NSe$
9-(Selenocyanato)fluorene, S-80025

$C_{14}H_9N_3$
4,4′-Iminobisbenzonitrile, *in* I-60018
5*H*-Indolo[2,3-*b*]quinoxaline, I-60036
Pyrido[2′,1′:2,3]imidazo[4,5-*c*]isoquinoline, P-60235
11*H*-Pyrimidino[4,5-*a*]carbazole, P-80225

$C_{14}H_9N_3O$
12*H*-Quinoxalino[2,3-*b*][1,4]benzoxazine, Q-70009

$C_{14}H_9N_3OS$
1,2,3-Benzotriazine-4(3*H*)-thione; *N*-Benzoyl, *in* B-60050

$C_{14}H_9N_3O_2$
5*H*-Indolo[2,3-*b*]quinoxaline; 5,11-Dioxide, *in* I-60036

$C_{14}H_9N_3S$
12*H*-Quinoxalino[2,3-*b*][1,4]benzothiazine, Q-70008

$C_{14}H_9N_3S_2$
Di-2-benzothiazolylamine, D-80074

$C_{14}H_{10}$
1-Benzylidene-1*H*-cyclopropabenzene, B-70084
Cyclohepta[*de*]naphthalene, C-60198
2,3-Dihydro-1,2,3-metheno-1*H*-phenalene, D-80218
2,12-Tetradecadiene-4,6,8,10-tetrayne, T-80029

$C_{14}H_{10}BrN$
1-(Bromomethyl)acridine, B-70229
2-(Bromomethyl)acridine, B-70230
3-(Bromomethyl)acridine, B-70231
4-(Bromomethyl)acridine, B-70232
9-(Bromomethyl)acridine, B-70233

$C_{14}H_{10}IN$
▷ 1*H*-Indol-3-ylphenyliodonium hydroxide inner salt, I-70017

$C_{14}H_{10}N_2$
10*b*,10*c*-Diazadicyclopenta[*ef*,*kl*]heptalene, D-70052

$C_{14}H_{10}N_2O$
9-Acridinecarboxaldehyde; Oxime, *in* A-70060
9-Acridinecarboxylic acid; Amide, *in* A-70061
3,5-Diphenyl-1,2,4-oxadiazole, D-60484
3-Nitroso-2-phenylindole, *in* P-60114
1*H*-Pyrrolo[3,2-*b*]pyridine; *N*-Benzoyl, *in* P-60249

$C_{14}H_{10}N_2O_2$
1,3-Diazetidine-2,4-dione; 1,3-Di-Ph, *in* D-60057
3,5-Diphenyl-1,2,4-oxadiazole; 4-Oxide, *in* D-60484
3-Methyl-1-phenazinecarboxylic acid, M-80136
4-Methyl-1-phenazinecarboxylic acid, M-80137
6-Methyl-1-phenazinecarboxylic acid, M-80138
7-Methyl-1-phenazinecarboxylic acid, M-80139
8-Methyl-1-phenazinecarboxylic acid, M-80140
9-Methyl-1-phenazinecarboxylic acid, M-80141
2-Phenylisatogen oxime, *in* P-60114

$C_{14}H_{10}N_2O_3$
N-(3-Oxo-3*H*-phenoxazin-2-yl)acetamide, *in* A-60237

$C_{14}H_{10}N_2O_4$
(4-Nitrophenyl)phenylethanedione; Monoxime, *in* N-70059
(2-Nitrophenyl)phenylethanedione; 1-Oxime, *in* N-70058
(2-Nitrophenyl)phenylethanedione; 2-Oxime, *in* N-70058

$C_{14}H_{10}N_2O_5$
4-Amino-2,6-pyridinedicarboxylic acid; *N*-Benzoyl, *in* A-70194

$C_{14}H_{10}N_2S$
3-Cyano-10-methylphenothiazine, *in* P-70057

$C_{14}H_{10}N_2Se$
3,4-Diphenyl-1,2,5-selenadiazole, D-70497

$C_{14}H_{10}O$
1-Acetylbiphenylene, A-80018
2-Acetylbiphenylene, A-80019
Benzo[5,6]cycloocta[1,2-*c*]furan, B-70029
9*H*-Fluorene-1-carboxaldehyde, F-70014
▷ 9*H*-Fluorene-9-carboxaldehyde, F-70015
8,1-[1]Propen[1]yl[3]ylidene-1*H*-benzocyclohepten-4(9*H*)-one, M-70042

$C_{14}H_{10}OS$
Dibenzo[*b*,*e*]thiepin-11(6*H*)-one, D-80075

$C_{14}H_{10}O_2$
2-Acetylnaphtho[1,8-*bc*]pyran, A-70048
1-Biphenylenecarboxylic acid; Me ester, *in* B-80109
2-Biphenylenecarboxylic acid; Me ester, *in* B-80110
1,3-Di(2-furyl)benzene, D-70168
1,4-Di(2-furyl)benzene, D-70169
3,4-Heptafulvalenedione, H-60022
4-Hydroxyacenaphthylene; Ac, *in* H-70100
4,5-Phenanthrenediol, P-70048

$C_{14}H_{10}O_3$
2-Benzoylbenzoic acid, B-80054
Disalicylaldehyde, D-70505
Naphtho[1,8-*bc*]pyran-2-carboxylic acid; Me ester, *in* N-70010
2,3,7-Phenanthrenetriol, T-60339
2,4,5-Phenanthrenetriol, P-60071
2,4,7-Phenanthrenetriol, P-80080

$C_{14}H_{10}O_4$
3,4-Acenaphthenedicarboxylic acid, A-60013
5,6-Acenaphthenedicarboxylic acid, A-70015
2,5-Dihydroxy-4-methoxy-9*H*-fluoren-9-one, *in* T-70261
2-(2,4-Dihydroxyphenyl)-6-hydroxybenzofuran, D-80363
2-Hydroxybenzoic acid; Benzoyl, *in* H-70108
2-Hydroxy-1-methoxyxanthone, *in* D-70353
6-(3,4-Methylenedioxystyryl)-α-pyrone, M-80086
Moracin *M*, M-60146
1,2,5,6-Tetrahydroxyphenanthrene, T-60115
1,2,5,7-Tetrahydroxyphenanthrene, T-80114
1,2,6,7-Tetrahydroxyphenanthrene, T-60117
1,3,5,6-Tetrahydroxyphenanthrene, T-60118
1,3,6,7-Tetrahydroxyphenanthrene, T-60119
2,3,4,7-Tetrahydroxyphenanthrene, T-80115
2,3,5,7-Tetrahydroxyphenanthrene, T-60120
2,3,6,7-Tetrahydroxyphenanthrene, T-60121
2,4,5,6-Tetrahydroxyphenanthrene, T-60122
3,4,5,6-Tetrahydroxyphenanthrene, T-60123

$C_{14}H_{10}O_4S$
2,2′-Thiobisbenzoic acid, T-70174
4,4′-Thiobisbenzoic acid, T-70175

$C_{14}H_{10}O_5$
▷ 1,3-Dihydroxy-7-methoxyxanthone, *in* T-80347
1,5-Dihydroxy-6-methoxyxanthone, *in* T-60349
▷ 1,7-Dihydroxy-3-methoxyxanthone, *in* T-80347
3,7-Dihydroxy-1-methoxyxanthone, *in* T-80347
5,6-Dihydroxy-1-methoxyxanthone, *in* T-60349
2-(2,4-Dihydroxyphenyl)-5,6-dihydroxybenzofuran, D-80355
6-Hydroxy-2-(2,3,4-trihydroxyphenyl)benzofuran, H-80260
1,2,5,6,7-Pentahydroxyphenanthrene, P-60050
1,3,4,5,6-Pentahydroxyphenanthrene, P-70034
2,3,4,7,9-Pentahydroxyphenanthrene, P-70035

$C_{14}H_{10}O_6$
2,5-Dihydroxy-1,4-naphthoquinone; Di-Ac, *in* D-60354
2,8-Dihydroxy-1,4-naphthoquinone; Di-Ac, *in* D-60355
5,8-Dihydroxy-1,4-naphthoquinone; Di-Ac, *in* D-60356
5,6-Dihydroxy-2-(2,3,4-trihydroxyphenyl)benzofuran, D-80389
1,2,3,5,6,7-Hexahydroxyphenanthrene, H-60066
2,4,5-Trihydroxy-1-methoxyxanthone, *in* T-70122

$C_{14}H_{10}O_6S$
4,4′-Sulfonylbisbenzoic acid, *in* T-70175

$C_{14}H_{10}S$
8-Methylthio-1,7-tridecadiene-3,5,9,11-tetrayne, M-80184
9-Phenanthrenethiol, P-70049

$C_{14}H_{10}S_2$
9,10-Dihydro-9,10-epidithioanthracene, D-70206

$C_{14}H_{10}S_3$
Benzenecarbodithioic acid anhydrosulfide, B-80013

$C_{14}H_{11}FO$
2-Fluoro-2,2-diphenylacetaldehyde, F-60033
3-Fluoro-4-methylphenol; Benzoyl, *in* F-60057

$C_{14}H_{11}FO_2$
2-Fluoro-3-hydroxybenzaldehyde; Benzyl ether, *in* F-60035
2-Fluoro-5-hydroxybenzaldehyde; Benzyl ether, *in* F-60036
4-Fluoro-3-hydroxybenzaldehyde; Benzyl ether, *in* F-60037

$C_{14}H_{11}IO_3S$
2-Iodo-1-phenyl-2-(phenylsulfonyl)ethanone, I-60061

$C_{14}H_{11}N$
1-Phenyl-1*H*-indole, P-70082
6-Phenyl-1*H*-indole, P-60113
N-Vinylcarbazole, V-80007

$C_{14}H_{11}NO$
1-Aminobiphenylene; N-Ac, *in* A-80062
2-Aminobiphenylene; N-Ac, *in* A-80063
9*H*-Fluorene-1-carboxaldehyde; Oxime, *in* F-70014
Isocyanatodiphenylmethane, I-80054
▷ *N*-Phenylphthalamidine, *in* P-70100

$C_{14}H_{11}NO_2$
1*H*-Benz[*e*]indole-1,2(3*H*)-dione; *N*-Et, *in* B-70026
2-Benzoylbenzoic acid; Amide, *in* B-80054
1-Hydroxycarbazole; Ac, *in* H-80137
2-Hydroxycarbazole; Ac, *in* H-60109

$C_{14}H_{11}NO_2S$
10*H*-Phenothiazine-1-carboxylic acid; *N*-Me, *in* P-70055
10*H*-Phenothiazine-2-carboxylic acid; *N*-Me, *in* P-70056
10*H*-Phenothiazine-3-carboxylic acid; *N*-Me, *in* P-70057
10*H*-Phenothiazine-4-carboxylic acid; *N*-Me, *in* P-70058
10*H*-Phenothiazine-1-carboxylic acid; Me ester, *in* P-70055
10*H*-Phenothiazine-2-carboxylic acid; Me ester, *in* P-70056

$C_{14}H_{11}NO_3S$
10*H*-Phenothiazine-1-carboxylic acid; Me ester, 5-oxide, *in* P-70055

$C_{14}H_{11}NO_4$
1,2-Dimethoxy-3*H*-phenoxazin-3-one, *in* T-60353
▷ 2,2′-Iminodibenzoic acid, I-60014
2,3′-Iminodibenzoic acid, I-60015
2,4′-Iminodibenzoic acid, I-60016
3,3′-Iminodibenzoic acid, I-60017
4,4′-Iminodibenzoic acid, I-60018

$C_{14}H_{11}NO_4S$
10*H*-Phenothiazine-1-carboxylic acid; *N*-Me, 5,5-dioxide, *in* P-70055
10*H*-Phenothiazine-2-carboxylic acid; *N*-Me, 5,5-dioxide, *in* P-70056
10*H*-Phenothiazine-3-carboxylic acid; *N*-Me, 5,5-dioxide, *in* P-70057
10*H*-Phenothiazine-4-carboxylic acid; *N*-Me, 5,5-dioxide, *in* P-70058
10*H*-Phenothiazine-2-carboxylic acid; Me ester, 5,5-dioxide, *in* P-70056

$C_{14}H_{11}N_3O_4$
(2-Nitrophenyl)phenylethanedione; Dioxime, *in* N-70058
(4-Nitrophenyl)phenylethanedione; Dioxime, *in* N-70059

$C_{14}H_{12}$
Biquadricyclenylidene, B-80131
9,10-Dihydrophenanthrene, D-60260
1,4-Dimethylbiphenylene, D-80424
1,5-Dimethylbiphenylene, D-80425
1,8-Dimethylbiphenylene, D-80426
2,3-Dimethylbiphenylene, D-80427
2,6-Dimethylbiphenylene, D-80428
2,7-Dimethylbiphenylene, D-80429
9*b*-Methyl-9*bH*-benz[*cd*]azulene, M-60044
Tricyclo[4.4.4.0^{1,6}]tetradeca-2,4,7,9,10,12-hexaene, T-70232

$C_{14}H_{12}Br_2$
1,2-Dibromo-1,2-diphenylethane, D-70091

$C_{14}H_{12}Br_2O_5$
3-Bromo-4-[(3-bromo-4,5-dihydroxyphenyl)methyl]-5-(hydroxymethyl)-1,2-benzenediol, B-70194

$C_{14}H_{12}ClNO_2$
2-Chloro-1-naphthylamine; *N*,*N*-Di-Ac, *in* C-80080

$C_{14}H_{12}N_2$
1,4-Dihydro-1,4-ethanonaphtho[1,8-*de*][1,2]diazepine, D-80207
1-Phenanthridenemethanamine, P-80081
10-Phenanthridinemethanamine, P-80083
4-Phenanthridinemethanamine, P-80082

$C_{14}H_{12}N_2O$
5,6-Dihydrobenzo[*c*]cinnoline; Mono-Ac, *in* D-80172
2,4-Dimethylcarbazole; *N*-Nitroso, *in* D-70382
3,6-Dimethylcarbazole; *N*-Nitroso, *in* D-70387
1,2-Diphenyl-1,2-diazetidin-3-one, *in* D-70055

$C_{14}H_{12}N_2O_2$
4,4′-Diamino-2,3′-biphenyldicarboxylic acid, D-80048
5,5′-Diamino-2,2′-biphenyldicarboxylic acid, D-80051
5*a*,6,11*a*,12-Tetrahydro[1,4]benzoxazino[3,2-*b*][1,4]benzoxazine, T-60059

$C_{14}H_{12}N_2O_4$
[2,2′-Bipyridine]-3,3′-dicarboxylic acid; Di-Me ester, *in* B-60124
[2,2′-Bipyridine]-3,5′-dicarboxylic acid; Di-Me ester, *in* B-60125
[2,2′-Bipyridine]-4,4′-dicarboxylic acid; Di-Me ester, *in* B-60126
[2,2′-Bipyridine]-5,5′-dicarboxylic acid; Di-Me ester, *in* B-60127
[3,3′-Bipyridine]-2,2′-dicarboxylic acid; Di-Me ester, *in* B-60133
[3,3′-Bipyridine]-4,4′-dicarboxylic acid; Di-Me ester, *in* B-60134
2,2′-Diamino-4,4′-biphenyldicarboxylic acid, D-80046
4,4′-Diamino-2,2′-biphenyldicarboxylic acid, D-80047
▷ 4,4′-Diamino-3,3′-biphenyldicarboxylic acid, D-80049
4,6′-Diamino-2,2′-biphenyldicarboxylic acid, D-80050

6,6′-Diamino-2,2′-biphenyldicarboxylic acid, D-80052
6,6′-Dihydroxy-2,2′-bipyridine; Di-Ac, *in* D-80299

$C_{14}H_{12}N_2S$
2-Amino-4*H*-3,1-benzothiazine; *N*-Ph, *in* A-70092
2,5-Dihydro-2,2-diphenyl-1,3,4-thiadiazole, D-60236

$C_{14}H_{12}N_4$
4-Amino-1,2,3-benzotriazine; 3-Benzyl, *in* A-60092
4-Amino-1,2,3-benzotriazine; *N*(4)-Benzyl, *in* A-60092
4-Amino-1,2,3-benzotriazine; 2-Me, *N*(4)-Ph, *in* A-60092
4-Amino-1,2,3-benzotriazine; 3-Me, *N*(4)-Ph, *in* A-60092

$C_{14}H_{12}N_4O_4$
Boxazomycin *B*, *in* B-70176
Boxazomycin *C*, *in* B-70176

$C_{14}H_{12}N_4O_5$
Boxazomycin *A*, B-70176

$C_{14}H_{12}N_4S$
3,5-Dianilino-1,2,4-thiadiazole, D-70048
Hector's base, H-60012

$C_{14}H_{12}O$
▷ 1-(Hydroxymethyl)fluorene, H-70176
1-Methoxyfluorene, *in* F-80016
1-Phenoxy-1-phenylethylene, *in* P-60092

$C_{14}H_{12}OS$
5,7-Dihydrodibenzo[*c*,*e*]thiepin; *S*-Oxide, *in* D-70190
9-(Methylsulfinyl)-9*H*-fluorene, *in* F-80015
2-(Methylthio)benzophenone, *in* M-70020
3-(Methylthio)benzophenone, *in* M-70021
4-(Methylthio)benzophenone, *in* M-70022
1-Phenyl-2-(phenylthio)ethanone, P-80120

$C_{14}H_{12}OS_2$
6*H*,12*H*-Dibenzo[*b*,*f*][1,5]dithiocin; *S*-Oxide, *in* D-70070
5*H*,7*H*-Dibenzo[*b*,*g*][1,5]dithiocin; 12-Oxide, *in* D-70069
5*H*,7*H*-Dibenzo[*b*,*g*][1,5]dithiocin; 6-Oxide, *in* D-70069

$C_{14}H_{12}OSe$
Phenyl styryl selenoxide, *in* P-70070

$C_{14}H_{12}O_2$
O-Acetylcapillol, *in* P-80104
1,2-Dihydrocyclobuta[*a*]naphthalene-2-carboxylic acid; Me ester, *in* D-70177
2,2′-Dihydroxystilbene, D-80378
2,4′-Dihydroxystilbene, D-80379
2,5-Dihydroxystilbene, D-80380
3,3′-Dihydroxystilbene, D-80381
3,4-Dihydroxystilbene, D-80382
3,4′-Dihydroxystilbene, D-80383
3,5-Dihydroxystilbene, D-80384
4,4′-Dihydroxystilbene, D-80385
1,2-Dimethoxybiphenylene, *in* B-80116
1,5-Dimethoxybiphenylene, *in* B-80117
2,3-Dimethoxybiphenylene, *in* B-80119
2,6-Dimethoxybiphenylene, *in* B-80120
2,7-Dimethoxybiphenylene, *in* B-80121
2-(2,4-Hexadiynylidene)-5-(propionylmethylidene)-2,5-dihydrofuran, H-80048
4-Hydroxyacenaphthene; Ac, *in* H-60099
2,3-Naphthalenedicarboxylic acid; Di-Me ester, *in* N-80001
1,2,3,4-Tetrahydroanthraquinone, T-60054

$C_{14}H_{12}O_2S$
4-[2,2′-Bithiophen-5-yl]-3-butyn-1-ol; Ac, *in* B-80167
5,7-Dihydrodibenzo[*c*,*e*]thiepin; *S*-Dioxide, *in* D-70190
9-(Methylsulfonyl)-9*H*-fluorene, *in* F-80015
1-Phenyl-2-(phenylsulfinyl)ethanone, *in* P-80120

$C_{14}H_{12}O_2S_2$
5*H*,7*H*-Dibenzo[*b*,*g*][1,5]dithiocin; 12,12-Dioxide, *in* D-70069

$C_{14}H_{12}O_2Se$
Phenyl styryl selenone, *in* P-70070

$C_{14}H_{12}O_3$
Demethylfrutescin, *in* H-80231
9,10-Dihydro-4-methoxy-2,7-phenanthrenediol, *in* P-80080
Isotriptospinocoumarin, I-80097
4′-Methoxy-2-biphenylcarboxylic acid, *in* H-70111
α-Oxo-1-naphthaleneacetic acid; Et ester, *in* O-60078
α-Oxo-2-naphthaleneacetic acid; Et ester, *in* O-60079
4-Phenoxybenzoic acid; Me ester, *in* P-80088
Triptispinocoumarin, T-80364

$C_{14}H_{12}O_3S$
1-Phenyl-2-(phenylsulfonyl)ethanone, *in* P-80120

$C_{14}H_{12}O_3S_2$
5-(3-Hydroxy-4-acetoxy-1-butynyl)-2,2′-bithienyl, *in* B-80166
5-(4-Hydroxy-3-acetoxy-1-butynyl)-2,2′-bithienyl, *in* B-80166

$C_{14}H_{12}O_4$
2,6-Azulenedicarboxylic acid; Di-Me ester, *in* A-70294
1,4-Dicarbomethoxyazulene, *in* A-70293
9,10-Dihydro-2,4,5,6-phenanthrenetetrol, D-70247
2,4-Dihydroxy-6-methoxybenzophenone, *in* T-80285
▷ 2,6-Dihydroxy-4-methoxybenzophenone, *in* T-80285
1-(2,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene, D-70335
1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene, D-80361
4′-Hydroxydehydrokawain, H-70122
1-(3-Hydroxyphenyl)-2-(2,4,5-trihydroxyphenyl)ethylene, H-70215
Osthenone, O-70049
Osthenone, O-80049
9-Tetradecene-2,4,6-triynedioic acid, T-80041

$C_{14}H_{12}O_4S_2$
5*H*,7*H*-Dibenzo[*b*,*g*][1,5]dithiocin; 6,6,12,12-Tetroxide, *in* D-70069

$C_{14}H_{12}O_5$
9,10-Dihydro-2,3,4,6,7-phenanthrenepentol, D-70246
1-(3,4-Dihydroxyphenyl)-2-(3,4,5-dihydroxyphenyl)ethylene, D-80360
▷ Khellin, K-60010

$C_{14}H_{12}O_6$
1-(2,3,4-Trihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethylene, T-60344

$C_{14}H_{12}O_8$
Fulvic acid, F-60081
Polivione, P-60167

$C_{14}H_{12}S$
5,7-Dihydrodibenzo[*c*,*e*]thiepin, D-70190
9-(Methylthio)-9*H*-fluorene, *in* F-80015

$C_{14}H_{12}S_2$
6*H*,12*H*-Dibenzo[*b*,*f*][1,5]dithiocin, D-70070
5*H*,7*H*-Dibenzo[*b*,*g*][1,5]dithiocin, D-70069

$C_{14}H_{12}Se$
5,7-Dihydrodibenzo[*c*,*e*]selenepin, D-70189
[(2-Phenylethenyl)seleno]benzene, P-70070

$C_{14}H_{13}N$
9-Amino-9,10-dihydroanthracene, A-60136
2-Amino-9,10-dihydrophenanthrene, A-60141
4-Amino-9,10-dihydrophenanthrene, A-60142
9-Amino-9,10-dihydrophenanthrene, A-60143
▷ 10,11-Dihydro-5*H*-dibenz[*b*,*f*]azepine, D-70185
1,2-Dimethylcarbazole, D-70374
1,3-Dimethylcarbazole, D-70375
1,4-Dimethylcarbazole, D-70376
1,5-Dimethylcarbazole, D-70377
1,6-Dimethylcarbazole, D-70378
1,7-Dimethylcarbazole, D-70379
1,8-Dimethylcarbazole, D-70380
2,3-Dimethylcarbazole, D-70381
2,4-Dimethylcarbazole, D-70382
2,5-Dimethylcarbazole, D-70383
2,7-Dimethylcarbazole, D-70384
3,4-Dimethylcarbazole, D-70385
3,5-Dimethylcarbazole, D-70386
3,6-Dimethylcarbazole, D-70387
4,5-Dimethylcarbazole, D-70388
2,2-Diphenylaziridine, D-80504

$C_{14}H_{13}NO$
1-Ethoxy-9*H*-carbazole, *in* H-80137
2-Ethoxycarbazole, *in* H-60109

$C_{14}H_{13}NO_2$
N-Acetoxy-4-aminobiphenyl, A-80013
4-Oxo-1,2,3,4-tetrahydrocarbazole; *N*-Ac, *in* O-70106

$C_{14}H_{13}NO_3$
(4-Hydroxyphenoxy)acetic acid; Anilide, *in* H-70205
3,4,6-Trihydroxy-1,2-dimethylcarbazole, T-70253

$C_{14}H_{13}NO_4$
6-Amino-2-hexenoic acid; *N*-Phthalimido, *in* A-60173
3-Amino-1,2-naphthalenediol; *O*,*O*-Di-Ac, *in* A-80116

$C_{14}H_{13}N_3O_2$
2,2′-Iminobisbenzamide, *in* I-60014

$C_{14}H_{14}$
Hexacyclo[6.5.1.0^{2,7}.0^{3,11}.0^{4,9}.0^{10,14}]tetradeca-5,12-diene, H-80039
Pentacyclo[8.4.0.0^{2,7}.0^{3,12}.0^{6,11}]tetradeca-4,8,13-triene, P-70021
1,2,3,4-Tetrahydroanthracene, T-60053
1,2,4,5-Tetravinylbenzene, T-80162

$C_{14}H_{14}N_2$
2,5-Dimethyl-3-(2-phenylethenyl)pyrazine, D-60442
N,*N*′-Diphenylformamidine; *N*-Me, *in* D-60479

$C_{14}H_{14}N_2O$
2,2′-Diaminobiphenyl; 2-*N*-Ac, *in* D-60033
N,*N*′-Diphenylurea; *N*-Me, *in* D-70499
5-Phenyl-3-pyridinecarboxylic acid; Dimethylamide, *in* P-80129

$C_{14}H_{14}N_2O_3S$
Sulfoacetic acid; Dianilide, *in* S-80050

$C_{14}H_{14}N_2O_5$
Antibiotic PDE II, A-70229

$C_{14}H_{14}N_2S_4$
2,2′-Bi(4,6-dimethyl-5*H*-1,3-dithiolo[4,5-*c*]pyrrolylidene), B-80092

$C_{14}H_{14}N_4$
5,5*a*,6,11,11*a*,12-Hexahydroquinoxalino[2,3-*b*]quinoxaline, H-80066

$C_{14}H_{14}N_4O_4$
4,4′-Diamino-3,3′-biphenyldicarboxylic acid; Diamide, *in* D-80049

$C_{14}H_{14}O$
2-(2-Phenylethyl)phenol, P-70071
3-(2-Phenylethyl)phenol, P-70072
4-(2-Phenylethyl)phenol, P-70073

$C_{14}H_{14}OS$
2-Mercaptobenzenemethanol; S-Benzyl, *in* M-80021
2-Mercapto-1,1-diphenylethanol, M-70028

$C_{14}H_{14}O_2$
3,4′-Dimethoxybiphenyl, *in* B-80106
2-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene, *in* H-70042
2,3,4,6,7,8-Hexahydro-1,5-anthracenedione, H-80051
1,2,3,6,7,8-Hexahydro-4,5-phenanthrenedione, H-80064
2,3,4,5,6,7-Hexahydro-1,8-phenanthrenedione, H-80065

1-Methoxy-2-(phenylmethoxy)benzene, *in* B-60072
1-Methoxy-3-(phenylmethoxy)benzene, *in* B-60073
1-Methoxy-4-(phenylmethoxy)benzene, *in* B-60074
2-(2-Phenylethyl)-1,4-benzenediol, P-60095
4-(2-Phenylethyl)-1,2-benzenediol, P-60096
4-(2-Phenylethyl)-1,3-benzenediol, P-60097
5-(2-Phenylethyl)-1,3-benzenediol, P-80100

$C_{14}H_{14}O_2S_2$
2-Mercaptobenzenemethanol; Disulfide, *in* M-80021
3-Mercaptobenzenemethanol; Disulfide, *in* M-80022
4-Mercaptobenzenemethanol; Disulfide, *in* M-80023

$C_{14}H_{14}O_3$
3,5-Dimethoxy-4-biphenylol, *in* B-80129
2-(Dimethoxymethyl)-1-naphthalenecarboxaldehyde, *in* N-60001
3-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid, D-50601
3-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid, D-70372
2-(2,4-Hexadiynylidene)-1,6-dioxaspira[4.5]dec-3-en-8-ol, H-70042
3,3′,4-Trihydroxybibenzyl, T-60316

$C_{14}H_{14}O_4$
1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethane, D-80359
5,8-Dihydroxy-2,3,6,7-tetramethyl-1,4-naphthoquinone, D-60377
1,4,5-Naphthalenetriol; 1,5-Di-Me ether, Ac, *in* N-60005
1,4,5-Naphthalenetriol; 4,5-Di-Me ether, Ac, *in* N-60005
Norpinguisanolide, N-80082
Phthalidochromene, P-60143
Platypodantherone, P-80161
Tenual, T-80007
3,3′,4,4′-Tetrahydroxybibenzyl, T-60101
3,3′,4,5-Tetrahydroxybibenzyl, T-60102

$C_{14}H_{14}O_5$
1-(3,4-Dihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethane, D-80371
Funadonin, F-70046
Haplopinol, *in* D-84287
Khellactone, K-70013
3,3′,4,4′,5-Pentahydroxybibenzyl, P-60044

$C_{14}H_{14}O_6$
3,3′,4,4′,5,5′-Hexahydroxybibenzyl, H-60062

$C_{14}H_{14}O_7$
3′,4′,5′-Trihydroxyacetophenone; Tri-Ac, *in* T-60315

$C_{14}H_{14}O_8$
1,2,3,4-Benzenetetrol; Tetra-Ac, *in* B-60014
Hexahydroxy-1,4-naphthoquinone; 2,3,6,7-Tetra-Me ether, *in* H-60065
3,4,5-Trihydroxyphenylacetic acid; Tri-Ac, *in* T-60343

$C_{14}H_{14}Se_2$
Dibenzyl diselenide, D-60082

$C_{14}H_{15}ClO_5$
Mikrolin, M-60135

$C_{14}H_{15}NO$
1,3,4,10-Tetrahydro-9(2*H*)-acridinone; *N*-Me, *in* T-60052

$C_{14}H_{15}NO_3$
1-Amino-2,7-naphthalenediol; Di-Me ether, *N*-Ac, *in* A-80113
4-Amino-1,2-naphthalenediol; Di-Me ether, N-Ac, *in* A-80117
4-Amino-1,5-naphthalenediol; Di-Me ether, N-Ac, *in* A-80119
5-Amino-2,3-naphthalenediol; Di-Me ether, N-Ac, *in* A-80122

$C_{14}H_{15}NO_4$
1*H*-Indole-3-carboxylic acid; *N*-COOEt, Et ester, *in* I-80012

$C_{14}H_{15}N_5O_4$
8-Aminoimidazo[4,5-*g*]quinazoline; 1-(β-D-Ribofuranosyl), *in* A-60207
lin-Benzoadenosine, *in* A-60207

$C_{14}H_{16}$
1,3-Diethynyladamantane, D-60172
Heptacyclo[6.6.0.0^{2,6}.0^{3,13}.0^{4,11}.0^{5,9}.0^{10,14}]tetradecane, H-70012
Heptacyclo[9.3.0.0^{2,5}.0^{3,13}.0^{4,8}.0^{6,10}.0^{9,12}]tetradecane, H-70013
1,2,3,9,10,10*a*-Hexahydrophenanthrene, H-80063

$C_{14}H_{16}N_2$
2,2′-Bis(methylamino)biphenyl, *in* D-60033
1,2-Diphenyl-1,2-ethanediamine, D-70480
1-(1-Naphthyl)piperazine, N-60013
1-(2-Naphthyl)piperazine, N-60014

$C_{14}H_{16}N_2O_2$
▷ 1,4-Bis(1-isocyanato-1-methylethyl)benzene, B-70149

$C_{14}H_{16}N_2O_3$
β-Methyltryptophan; *N*-Ac, *in* M-80187

$C_{14}H_{16}N_4$
5,6,8,9-Tetraaza[3.3]paracyclophane, T-60018

$C_{14}H_{16}O$
4,6,12-Tetradecatrien-8,10-diyn-1-ol, T-80032
5-Tetradecene-8,10,12-triyn-1-ol, T-80042
6-Tetradecene-8,10,12-triyn-3-ol, T-80043

$C_{14}H_{16}O_2$
8-Norlactaranelactone, N-80080
2-Phenacylcyclohexanone, P-70045
7-Phenyl-5-heptynoic acid; Me ester, *in* P-60106
4,6,12-Tetradecatriene-8,10-diyne-1,3-diol, T-80033

$C_{14}H_{16}O_3$
3-(3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid, *in* D-50601
Drupanin, D-80534

$C_{14}H_{16}O_4$
6-Acetyl-7-hydroxy-8-methoxy-2,2-dimethyl-2*H*-1-benzopyran, A-80023
7-Hydroxy-4-isopropyl-3-methoxy-6-methylcoumarin, H-70144
Pyriculol, P-60216

$C_{14}H_{16}O_5$
Dechloromikrolin, *in* M-60135

$C_{14}H_{16}O_6$
Gravolenic acid, G-80037
7-Methoxycaleteucrin, *in* C-80012
1,5,8-Trihydroxy-3-methoxyxanthone, *in* T-70123

$C_{14}H_{16}O_7$
3-Methyl-1,2,4,5-benzenetetrol; 1-Me ether, Tri-Ac, *in* M-80048
4-Methyl-1,2,3,5-benzenetetrol; 3-Me ether, tri-Ac, *in* M-80049
Sawaranin, S-70016

$C_{14}H_{16}O_8$
1,3,5,7-Adamantanetetracarboxylic acid, A-80037

$C_{14}H_{17}NO$
8-Azabicyclo[3.2.1]octane; *N*-Benzoyl, *in* A-70278

$C_{14}H_{17}NO_3$
3-Amino-4-hexenoic acid; *N*-Benzoyl, Me ester, *in* A-60171

$C_{14}H_{17}NO_9$
2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one; Demethoxy, 2-*O*-β-D-glucoside, *in* D-10388

$C_{14}H_{18}$
Benzylidenecycloheptane, B-60068
Tetrahydro-1,6,7-tris(methylene)-1*H*,4*H*-3*a*,6*a*-propanopentalene, T-70101

$C_{14}H_{18}N_2$
1,8-Bis(dimethylamino)naphthalene, *in* D-70042

$C_{14}H_{18}N_2O_5$
Aspartame, A-60311

$C_{14}H_{18}N_4O_4$
1,2,3,5-Tetraaminobenzene; *N*-Tetra-Ac, *in* T-60012
1,2,4,5-Tetraaminobenzene; 1,2,4,5-*N*-Tetra-Ac, *in* T-60013

$C_{14}H_{18}O$
3,4-Dihydro-3,3,6,8-tetramethyl-1(2*H*)-napthalenone, D-80254
Foeniculin, *in* P-80179
6,12-Tetradecadiene-8,10-diyn-3-ol, T-80028
4,6,10,12-Tetradecatetraen-8-yn-1-ol, T-80031
8-Tetradecene-11,13-diyn-2-one, T-80040

$C_{14}H_{18}O_2$
Anol isovalerate, *in* P-80179
Majusculone, M-70006
Norpinguisone, N-80083
4,6-Tetradecadiene-8,10-diyne-1,12-diol, T-80026
6,12-Tetradecadiene-8,10-diyne-1,3-diol, T-80027

$C_{14}H_{18}O_2S$
9-(2-Thienyl)-4,6-nonadien-8-yn-1-ol; Deoxy, 3-acetoxy, 4,5-dihydro, *in* T-80181

$C_{14}H_{18}O_3$
5-(1,3-Dihydroxypropyl)-2-isopropenyl-2,3-dihydrobenzofuran, D-70340
6-Ethoxy-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran, *in* D-70365

$C_{14}H_{18}O_4$
1-Acetyl-4-isopentenyl-6-methylphloroglucinol, *in* T-70248
11-Hydroxy-3-oxo-13-nor-7(11)-eudesmen-12,6-olide, H-60204
Hyperolactone, H-80267
3-Isopropyl-6-methyl-1,2-benzenediol; Di-Ac, *in* I-60124

$C_{14}H_{18}O_6$
Colletoketol, *in* C-60159

$C_{14}H_{18}O_7$
3,7*a*-Diacetoxyhexahydro-2-oxa-3*a*,7-dimethyl-1,4-indanedione, *in* H-70055

$C_{14}H_{19}NO_2$
2-(Aminomethyl)cyclohexanol; *N*-Benzoyl, *in* A-70169

$C_{14}H_{19}NO_7$
Menisdaurin, *in* L-70034

$C_{14}H_{19}NO_8$
Griffonin, *in* L-70034
Lithospermoside, L-70034
Lithospermoside; 5-Epimer, *in* L-70034
Thalictoside, *in* N-70050

$C_{14}H_{19}N_3$
1-Azidodiamantane, A-60341
3-Azidodiamantane, A-60342
4-Azidodiamantane, A-60343
2,3,5,6-Tetrahydro-1*H*,4*H*,7*H*,11*cH*-3*a*,6*a*,11*b*-triazabenz[*de*]anthracene, T-80079

$C_{14}H_{19}N_3O_4$
Citrulline; α-*N*-Benzoyl, Me ester, *in* C-60151

$C_{14}H_{20}$
7,7′-Bi(bicyclo[2.2.1]heptylidene), B-60078
1,2-Bis(cyclohexylidene)ethene, B-80144
1,3-Divinyladamantane, D-70529
1-Phenyl-1-octene, P-80106
1-Phenyl-2-octene, P-80107
2-Phenyl-1-octene, P-80108

$C_{14}H_{20}N_2$
3,6-Di-*tert*-butylpyrrolo[3,2-*b*]pyrrole, D-70108

$C_{14}H_{20}N_2O_4$
3-Methyl-*N*-(5*a*,6*a*,7,8-tetrahydro-4-methyl-1,5-dioxo-1*H*,5*H*-pyrrolo[1,2-*c*][1,3]oxazepin-3-yl)butanamide, M-70134

$C_{14}H_{20}N_6$
2,3,4,5,6,7,8,9,10,11-Decahydro-1,3*a*,5*a*,7*a*,9*a*,12-hexaazatricyclopenta[*a*,*ef*,*j*]heptalene, D-80011

$C_{14}H_{20}N_6O_4S_2$
5,5′-Dithiobis[1-methylhistidine], *in* M-80025

$C_{14}H_{20}O_2$
1,3-Epoxy-2-nor-1,10-seco-1(5),3-aromadendradien-10-one, E-80041
1,3,5,7-Tetramethyl-2,4-adamantanedione, T-60131

$C_{14}H_{20}O_3$
Ceratenolone, C-60030
2,4-Dimethyl-1,3-pentanediol; 3-*O*-Benzoyl, *in* D-80466
7-Oxo-11-nordrim-8-en-12-oic acid, O-60080

$C_{14}H_{20}O_5$
Seiricuprolide, S-70028
Wasabidienone *A*, W-70001

$C_{14}H_{20}O_6$
Colletodiol, C-60159

$C_{14}H_{20}O_8$
Ethylenetetracarboxylic acid; Tetra-Et ester, *in* E-60049

$C_{14}H_{20}O_{10}$
1,2,5,6-Tetra-*O*-acetyl-*myo*-inositol, *in* I-80015

$C_{14}H_{20}S_6$
1,3,4,6-Tetrakis(ethylthio)thieno[3,4-*b*]thiophene, *in* T-70170

$C_{14}H_{21}N$
[9](2,6)Pyridinophane, P-80214

$C_{14}H_{21}NO$
1,2,3,4,5,6,7,8,8*a*,9*a*-Decahydrocarbazole; *N*-Ac, *in* D-70012
[9](2,6)Pyridinophane; *N*-Oxide, *in* P-80214

$C_{14}H_{21}NO_3$
4,5-Dihydroxy-2-methylbenzoic acid; Di-Me ether, *N*,*N*-diethylamide, *in* D-80339

$C_{14}H_{21}NO_4$
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid; 1-Me, di-Et ester, *in* D-80193
Wasabidienone *D*, W-70002

$C_{14}H_{22}$
1,1,2,2-Tetracyclopropylethane, T-60034

$C_{14}H_{22}N_2$
Bis(1,1-dicyclopropylmethyl)diazene, B-60154
1,4-Dihydropyrrolo[3,2-*b*]pyrrole; 1,4-Di-*tert*-butyl, *in* D-30286

$C_{14}H_{22}N_6O_3$
3′-Amino-3′-deoxyadenosine; 3′,3′,6,6-Tetra-*N*-Me, *in* A-70128

$C_{14}H_{22}O$
Norpatchoulenol, N-70078
5,7,9,11-Tetradecatetraen-1-ol, T-80030
1,3,5,7-Tetramethyladamantanone, T-60132

$C_{14}H_{22}O_2$
Sulcatine, S-60061

$C_{14}H_{22}O_3$
5,7-Dihydroxy-13-nor-8-marasmanone, D-60361
5,8-Dihydroxy-13-nor-7-marasmanone, D-60362
6-Hydroxy-2,4,8-tetradecatrienoic acid, H-70222

$C_{14}H_{22}O_5$
Botrylactone, B-70174

$C_{14}H_{23}N_3O_2$
1*H*-Pyrrole-3,4-dicarboxylic acid; Diethylamide, *in* P-70183

$C_{14}H_{24}$
1,8-Cyclotetradecadiene, C-70252

$C_{14}H_{24}N_2O_{10}$
▷ 3,12-Bis(carboxymethyl)-6,9-dioxa-3,12-diazatetradecanedioic acid, B-70134

$C_{14}H_{24}N_6$
1,3,4,6-Tetrakis(dimethylamino)pyrrolo[3,4-*c*]pyrrole, T-70127

$C_{14}H_{24}O$
4-Cyclotetradecen-1-one, C-80198
5-Cyclotetradecen-1-one, C-80199

$C_{14}H_{24}O_2$
11-Dodecyn-1-ol; Ac, *in* D-70540
5-Tetradecen-13-olide, T-80045
12-Tetradecen-14-olide, *in* H-60230

$C_{14}H_{24}O_8$
Rengyoside *B*, *in* R-80004

$C_{14}H_{26}$
1,1,2,2,3,3,4,4-Octamethyl-5-methylenecyclopentane, O-60027

$C_{14}H_{26}BBrF_4N_2$
Bis(quinuclidine)bromine(1+); Tetrafluoroborate, *in* B-60173

$C_{14}H_{26}BrN_2^{\oplus}$
Bis(quinuclidine)bromine(1+), B-60173

$C_{14}H_{26}Br_2N_2$
Bis(quinuclidine)bromine(1+); Bromide, *in* B-60173

$C_{14}H_{26}N_4$
1,2,4,5-Tetrakis(dimethylamino)benzene, *in* T-60012
1,2,4,5-Tetrakis(dimethylamino)benzene, *in* T-60013

$C_{14}H_{26}O$
6-Isopropenyl-3-methyl-9-decen-1-ol, I-70089
7-Tetradecyn-1-ol, T-60042

$C_{14}H_{26}O_2$
9-Dodecen-1-ol; Ac, *in* D-70537
3-Tetradecenoic acid, T-80044

$C_{14}H_{26}O_3$
12-Hydroxy-13-tetradecenoic acid, H-60229
14-Hydroxy-12-tetradecenoic acid, H-60230

$C_{14}H_{26}O_8$
Rengyoside A, R-80004

$C_{14}H_{28}$
Cyclotetradecane, C-70253
2-Tetradecene, T-80034
3-Tetradecene, T-80035
4-Tetradecene, T-80036
5-Tetradecene, T-80037
6-Tetradecene, T-80038
7-Tetradecene, T-80039

$C_{14}H_{28}NO_2^{\oplus}$
1,1-*tert*-Butyl-3,3-diethoxy-2-azaallenium(1+), B-70301

$C_{14}H_{28}N_2O_5$
Levocarnitine; Dimeric intermolecular ester, *in* C-70024

$C_{14}H_{28}O$
Nonamethylcyclopentanol, N-60057
5-Tetradecanone, T-60039

$C_{14}H_{28}O_3$
9-Hydroxydecanoic acid; *tert*-Butyl ester, *in* H-80149

$C_{14}H_{28}O_4$
3,9-Dihydroxytetradecanoic acid, D-80386

$C_{14}H_{30}$
3,4-Diisopropyl-2,5-dimethylhexane, D-60393

$C_{14}H_{30}O$
4,6,8-Trimethyl-2-undecanol, T-60372

$C_{14}H_{31}N_3O_3$
1,7,14-Trioxa-4,11,17-triazacycloeicosane, T-80357

$C_{14}H_{33}N_5$
1,4,8,12,16-Pentaazacyclononadecane, P-60022

$C_{14}K_2N_6O_2$
Croconate blue, *in* T-70321

$C_{14}N_6O_2$
2,4,5-Tris(dicyanomethylene)-1,3-cyclopentanedione, T-70321

$C_{15}H_7Cl_2F_3N_2O_2$
▷ Phenyl 5,6-dichloro-2-(trifluoromethyl)-1*H*-benzimidazole-1-carboxylate, *in* D-60160

$C_{15}H_8ClNS$
4-Chloro-10*H*-phenothiazine, C-60127

$C_{15}H_8Cl_2O_5$
3′,6-Dichloro-4′,5,7-trihydroxyisoflavone, D-80147

$C_{15}H_8N_4S_2$
13*H*-[1,3,5]Thiadiazino[3,2-*a*:5,6-*a*′]bisbenzimidazole-13-thione, T-60191

$C_{15}H_8O_2$
5*H*-Phenanthro[4,5-*bcd*]pyran-5-one, *in* H-80232

$C_{15}H_8O_4$
Benzophenone-2,2′-dicarboxylic acid; Anhydride, *in* B-70041

$C_{15}H_8O_6$
2,3,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, T-70249
2,3,9-Trihydroxycoumestan, T-80293
3,7,9-Trihydroxycoumestan, T-80294
3,8,9-Trihydroxycoumestan, T-80295
5,9,10-Trihydroxy-2*H*-pyrano[2,3,4-*kl*]xanthen-2-one, T-70273

$C_{15}H_8O_7$
1,3,8,9-Tetrahydroxycoumestan, T-80087
2,3,8,9-Tetrahydroxycoumestan, T-80088
3,4,8,9-Tetrahydroxycoumestan, T-80089

$C_{15}H_8O_8$
1,2,3,8,9-Pentahydroxycoumestan, P-80029

$C_{15}H_9ClO_5$
6-Chloro-4′,5,7-trihydroxyisoflavone, C-80120

$C_{15}H_9IO_2$
3-Iodo-2-phenyl-4*H*-1-benzopyran-4-one, I-60059

$C_{15}H_9N$
Cyclohepta[*def*]carbazole, C-70220
2-(Phenylethynyl)benzoic acid; Nitrile, *in* P-70074

$C_{15}H_9NO_2$
3-Phenyl-1,4-isoquinolinedione, P-70083

$C_{15}H_9NO_3$
Benzophenone-2,2′-dicarboxylic acid; Imide, *in* B-70041

$C_{15}H_9NS$
[1]Benzothieno[3,2-*b*]quinoline, B-70063
[1]Benzothieno[2,3-*c*]quinoline, B-70062
[1]Benzothieno[3,2-*c*]quinoline, B-70064

$C_{15}H_9N_3O$
Indolo[2,3-*b*][1,4]benzodiazepin-12(6*H*)-one, I-70015

$C_{15}H_{10}$
▷ 4*H*-Cyclopenta[*def*]phenanthrene, C-70244
1*H*-Cyclopropa[*l*]phenanthrene, C-80197

$C_{15}H_{10}BF_4N$
Cyclohepta[*def*]carbazolium tetrafluoroborate, *in* C-70220

$C_{15}H_{10}ClN_3$
5-Chloro-4,6-diphenyl-1,2,3-triazine, C-80054

$C_{15}H_{10}Cl_2O_5$
Thiomelin, T-70181

$C_{15}H_{10}F_6NP$
Isoindolo[1,2,3-*de*]quinolizinium(1+); Hexafluorophosphate, *in* I-80064

$C_{15}H_{10}N^{\oplus}$
Isoindolo[1,2,3-*de*]quinolizinium(1+), I-80064

$C_{15}H_{10}N_2$
5*H*-Cyclohepta[4,5]pyrrolo[2,3-*b*]indole, C-60200
Indazolo[3,2-*a*]isoquinoline, I-60020
10*H*-Indolo[3,2-*b*]quinoline, I-70016
2-Methylbenzo[*gh*]perimidine, M-60051

$C_{15}H_{10}N_2O$
10*H*-Indolo[3,2-*b*]quinoline; 5-Oxide, *in* I-70016

$C_{15}H_{10}N_2O_2$
2-Diazo-1,3-diphenyl-1,3-propanedione, D-70058

$C_{15}H_{10}N_8OS_2$
S,S'-Bis(1-phenyl-1*H*-tetrazol-5-yl) dithiocarbonate, B-70155

$C_{15}H_{10}O_2$
1-Acetoxy-7-phenyl-2,4,6-heptatriyne, *in* P-80101
1-Acetoxy-2,12-tridecadiene-4,6,8,10-tetrayne, *in* T-80253
2-(Phenylethynyl)benzoic acid, P-70074
4-(Phenylethynyl)benzoic acid, P-70075

$C_{15}H_{10}O_2S$
Dibenzo[*b,f*]thiepin-3-carboxylic acid, D-60077
3-Mercapto-2-phenyl-4*H*-1-benzopyran-4-one, M-60025
2-Phenyl-4*H*-1-benzothiopyran-4-one; *S*-Oxide, *in* P-60082

$C_{15}H_{10}O_3$
6-Hydroxyflavone, H-70130
7-Hydroxyflavone, H-70131
▷ 8-Hydroxyflavone, H-70132
1-Hydroxy-7-methylanthraquinone, H-60170
5-Hydroxy-4-phenanthrenecarboxylic acid, H-80232
3-(3-Hydroxyphenyl)-1*H*-2-benzopyran-1-one, H-70207

$C_{15}H_{10}O_3S$
2-Phenyl-4*H*-1-benzothiopyran-4-one; *S,S*-Dioxide, *in* P-60082

$C_{15}H_{10}O_4$
4',6-Dihydroxyaurone, D-80273
2',8-Dihydroxyflavone, D-70300
4',7-Dihydroxyisoflavone, D-80323
3,9-Dihydroxypterocarpene, D-80376

$C_{15}H_{10}O_4S$
Dibenzo[*b,f*]thiepin-3-carboxylic acid; 5,5-Dioxide, *in* D-60077

$C_{15}H_{10}O_5$
Benzophenone-2,2'-dicarboxylic acid, B-70041
Chalaurenol, C-70036
▷ 1,3-Dihydroxy-2-hydroxymethylanthraquinone, D-70306
3-(2,4-Dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran-2-one, D-80364
2-(2,4-Dihydroxyphenyl)-5,6-methylenedioxybenzofuran, *in* D-80355
Nivegin, N-80063
Sulfuretin, S-70082
2',5,5'-Trihydroxyflavone, T-80298
3,4',7-Trihydroxyflavone, T-80300
3',4',7-Trihydroxyflavone, T-80301
5,6,7-Trihydroxyflavone, T-60322
2',4',7-Trihydroxyisoflavone, T-70264
2',4',7-Trihydroxyisoflavone, T-80306
2',5,7-Trihydroxyisoflavone, T-80307
3',4',7-Trihydroxyisoflavone, T-80308
▷ 4',5,7-Trihydroxyisoflavone, T-80309
4',6,7-Trihydroxyisoflavone, T-80310
4',7,8-Trihydroxyisoflavone, T-70265
4',7,8-Trihydroxyisoflavone, T-80311
1,2,7-Trihydroxy-6-methylanthraquinone, T-70268
1,2,8-Trihydroxy-3-methylanthraquinone, T-80322
1,6,8-Trihydroxy-2-methylanthraquinone, T-70269
Vertixanthone, *in* H-80266

$C_{15}H_{10}O_6$
Aureusidin, A-80188
4-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2*H*-1-benzopyran-2-one, D-70334
4-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2*H*-1-benzopyran-2-one, D-80356
7-Hydroxy-3-(2,4,5-trihydroxyphenyl)-2*H*-1-benzopyran-2-one, H-80261
Hydroxyvertixanthone, *in* H-80266
3',4',5,6,7-Pentahydroxyisoflavone, P-80043
2',3',5,7-Tetrahydroxyflavone, T-60106
2',5,6,6'-Tetrahydroxyflavone, T-70107
2',5,6',7-Tetrahydroxyflavone, T-50153
3',4',5,6-Tetrahydroxyflavone, T-70108
3',4',6,7-Tetrahydroxyflavone, T-80092
3',4',6,7-Tetrahydroxyisoflavanone, T-80102
2',3',4',7-Tetrahydroxyisoflavone, T-80105
2',4',5,7-Tetrahydroxyisoflavone, T-80106
2',4',5',7-Tetrahydroxyisoflavone, T-80107
2',5,6,7-Tetrahydroxyisoflavone, T-60107
2',5,6,7-Tetrahydroxyisoflavone, T-80108
2',5,7,8-Tetrahydroxyisoflavone, T-70110
3',4',5,7-Tetrahydroxyisoflavone, T-80109
3',4',5',7-Tetrahydroxyisoflavone, T-80110
3',4',7,8-Tetrahydroxyisoflavone, T-70112
4',5,6,7-Tetrahydroxyisoflavone, T-80112
4',5,7,8-Tetrahydroxyisoflavone, T-80113
4',6,7,8-Tetrahydroxyisoflavone, T-70113
1,3,4,5-Tetrahydroxy-2-methylanthraquinone, T-60112
1,3,5,8-Tetrahydroxy-2-methylanthraquinone, T-60113
3,4,8,9-Tetrahydroxypterocarpene, T-80122

$C_{15}H_{10}O_7$
4-(3,4-Dihydroxyphenyl)-5,7,8-trihydroxycoumarin, D-80370
2',3',4',5,6-Pentahydroxyflavone, P-70030
2',3,5,7,8-Pentahydroxyflavone, P-70029
2',4',5,5',7-Pentahydroxyflavone, P-80033
2',4',5,7,8-Pentahydroxyflavone, P-80034
3,4',5,6,7-Pentahydroxyflavone, P-80035
3,4',5,6,8-Pentahydroxyflavone, P-60048
3,5,6,7,8-Pentahydroxyflavone, P-70031
2',4',5,5',7-Pentahydroxyisoflavone, P-80041
2',4',5',6,7-Pentahydroxyisoflavone, P-80042
3',4',5,6,7-Pentahydroxyisoflavone, P-70032
3',4',5',6,7-Pentahydroxyisoflavone, P-80044
3',4',5,7,8-Pentahydroxyisoflavone, P-80045
3',4',6,7,8-Pentahydroxyisoflavone, P-80046

$C_{15}H_{10}O_8$
2',3,3',5,7,8-Hexahydroxyflavone, H-70079
2',3,5,5',6,7-Hexahydroxyflavone, H-60064
2',3,5,5',7,8-Hexahydroxyflavone, H-70080
3,3',4',5,6,7-Hexahydroxyflavone, H-80067
3',4',5,5',6,7-Hexahydroxyflavone, H-70081
2',4',5,5',6,7-Hexahydroxyisoflavone, H-80069
2',4',5,5',7,8-Hexahydroxyisoflavone, H-80070
3',4',5,5',6,7-Hexahydroxyisoflavone, H-80071

$C_{15}H_{10}O_9$
3,3',4',5,5',7,8-Heptahydroxyflavone, H-70021
3,3',4',5,6,7,8-Heptahydroxyflavone, H-80028
3',4',5,5',6,7,8-Heptahydroxyflavone, H-80029

$C_{15}H_{10}O_{10}$
2',3,4',5,5',6,7,8-Octahydroxyflavone, O-60022
3,3',4',5,5',6,7,8-Octahydroxyflavone, O-70018

$C_{15}H_{11}^{\oplus}$
Dibenzo[*a,d*]cycloheptenylium, D-60071

$C_{15}H_{11}Br$
1-(Bromomethyl)phenanthrene, B-80224
2-(Bromomethyl)phenanthrene, B-80225
3-(Bromomethyl)phenanthrene, B-80226
9-(Bromomethyl)phenanthrene, B-80227

$C_{15}H_{11}Cl$
1-(Chloromethyl)phenanthrene, C-80073
2-(Chloromethyl)phenanthrene, C-80074
3-(Chloromethyl)phenanthrene, C-80075
4-(Chloromethyl)phenanthrene, C-80076
9-(Chloromethyl)phenanthrene, C-80077

$C_{15}H_{11}ClN_2O_2$
2-Chloro-2,3-dihydro-1*H*-imidazole-4,5-dione; 1,3-Di-Ph, *in* C-60054

$C_{15}H_{11}ClO_2S$
2-(3-Chloro-4-acetoxy-1-butynyl)-5-(1,3-pentadiynyl)thiophene, *in* P-80025

$C_{15}H_{11}ClO_4$
Dibenzo[*a,d*]cycloheptenylium; Perchlorate, *in* D-60071

$C_{15}H_{11}ClO_5$
2-Chloro-1,8-dihydroxy-5-methoxy-6-methylxanthone, *in* T-70181
3,4',5,7-Tetrahydroxyflavylium; Chloride, *in* T-80093

$C_{15}H_{11}ClO_6$
3',4',5,5',7-Pentahydroxyflavylium; Chloride, *in* P-80036
3',4',5,7,8-Pentahydroxyflavylium; Chloride, *in* P-80037

$C_{15}H_{11}N$
5,10-Dihydroindeno[1,2-*b*]indole, D-80216

$C_{15}H_{11}NO$
6-Benzoylindole, B-60058
8-Hydroxy-7-phenylquinoline, H-60218
2-(Phenylethynyl)benzoic acid; Amide, *in* P-70074
2-Phenyl-4(1*H*)-quinolinone, P-60132
4-Phenyl-2(1*H*)-quinolinone, P-60131

$C_{15}H_{11}NOS$
▷ 2-Phenyl-1,5-benzothiazepin-4(5*H*)-one, P-60081

$C_{15}H_{11}NO_2$
▷ 9-Acridinecarboxylic acid; Me ester, *in* A-70061
10-Amino-9-anthracenecarboxylic acid, A-70088
Dibenz[*b,g*]azocine-5,7(6*H*,12*H*)-dione, D-60068
2,4-Diphenyl-5(4*H*)-oxazolone, D-60485
▷ 3-Nitro-1,2-diphenylcyclopropene, N-80046

$C_{15}H_{11}NO_3$
▷ 1-Amino-2-methoxyanthraquinone, *in* A-60174
▷ 1-Amino-4-methoxyanthraquinone, *in* A-60175
1-Amino-5-methoxyanthraquinone, *in* A-60176
9-Amino-10-methoxy-1,4-anthraquinone, *in* A-60181
1-Hydroxy-4-(methylamino)anthraquinone, *in* A-60175

$C_{15}H_{11}NO_3S$
10*H*-Phenothiazine-2-carboxylic acid; *N*-Ac, *in* P-70056

$C_{15}H_{11}NS$
10*H*-[1]Benzothieno[3,2-*b*]indole; *N*-Me, *in* B-70059
2-(2-Phenylethenyl)benzothiazole, P-60093
3-Phenyl-2(1*H*)-quinolinethione, P-80133

$C_{15}H_{11}N_3$
1-Phenyl-1*H*-pyrazolo[3,4-*e*]indolizine, P-70092

$C_{15}H_{11}O_2^{\oplus}$
2,5-Diphenyl-1,3-dioxol-1-ium, D-70478

$C_{15}H_{11}O_5^{\oplus}$
3,4',5,7-Tetrahydroxyflavylium, T-80093

$C_{15}H_{11}O_6^{\oplus}$
3',4',5,5',7-Pentahydroxyflavylium, P-80036
3',4',5,7,8-Pentahydroxyflavylium, P-80037

$C_{15}H_{12}$
3-Methylphenanthrene, M-70108

$C_{15}H_{12}I_3NO_4$
3,3',5-Triiodothyronine, T-60350

$C_{15}H_{12}N_2O$
2-Amino-4,5-diphenyloxazole, A-80068
4-Amino-2,5-diphenyloxazole, A-80069
5-Amino-2,4-diphenyloxazole, A-80070
5-Amino-3-phenylisoxazole; *N*-Ph, *in* A-60240
2-Methyl-1*H*-pyrrolo[2,3-*b*]pyridine; *N*-Benzoyl, *in* M-80156

$C_{15}H_{12}N_2O_2$
4-Methyl-1-phenazinecarboxylic acid; Me ester, *in* M-80137
6-Methyl-1-phenazinecarboxylic acid; Me ester, *in* M-80138

8-Methyl-1-phenazinecarboxylic acid; Me ester, *in* M-80140
9-Methyl-1-phenazinecarboxylic acid; Me ester, *in* M-80141
3,5-Pyrazolidinedione; 1,2-Di-Ph, *in* P-80200

$C_{15}H_{12}N_2O_3$
2,3-Dihydro-2-hydroxy-1*H*-imidazole-4,5-dione; 1,3-Di-Ph, *in* D-60243

$C_{15}H_{12}O$
5,7-Dihydro-6*H*-dibenzo[*a*,*c*]cyclohepten-6-one, D-70187
6,7-Dihydro-5*H*-dibenzo[*a*,*c*]cyclohepten-5-one, D-70188
10,11-Dihydro-5*H*-dibenzo[*a*,*d*]cyclohepten-5-one, D-60218
9-Phenanthrenemethanol, P-80079

$C_{15}H_{12}OS$
2,3-Dihydro-2-phenyl-4*H*-1-benzothiopyran-4-one, D-70248
1,2-Dimethylthioxanthone, D-70440
1,3-Dimethylthioxanthone, D-70441
1,4-Dimethylthioxanthone, D-70442
2,3-Dimethylthioxanthone, D-70443
2,4-Dimethylthioxanthone, D-70444
3,4-Dimethylthioxanthone, D-70445
3-Hydroxymethyldibenzo[*b*,*f*]thiepin, H-60176

$C_{15}H_{12}O_2$
2,7-Dimethylxanthone, D-60453
(4-Hydroxyphenyl)ethylene; Benzoyl, *in* H-70209

$C_{15}H_{12}O_2S$
1-Acetoxy-4-[5-(1,3-pentadiynyl)-2-thienyl]-3-butyne, *in* P-80025
2-(1-Acetoxy-3-penten-1-ynyl)-5-(3-buten-1-ynyl)thiophene, *in* B-80281
2,3-Dihydro-2-phenyl-4*H*-1-benzothiopyran-4-one; 1-Oxide, *in* D-70248

$C_{15}H_{12}O_2S_2$
5-Acetoxymethyl-5′-(3-buten-1-ynyl)-2,2′-bithienyl, *in* B-80279

$C_{15}H_{12}O_3$
7-(3-Acetoxyphenyl)-2-heptene-4,6-diyn-1-ol, *in* H-80234
2-Benzoylbenzoic acid; Me ester, *in* B-80054
2,7-Biphenylenediol; Me ether, Ac, *in* B-80121
1,3-Bis(4-hydroxyphenyl)-2-propen-1-one, B-80152
3,4-Dihydro-3-(3-hydroxyphenyl)-1*H*-2-benzopyran-1-one, *in* H-70207
2,3-Dihydro-2-phenyl-2-benzofurancarboxylic acid, D-60262
1-(2-Hydroxyphenyl)-3-phenyl-1,3-propanedione, H-80239
4-Methoxy-2,5-phenanthrenediol, *in* P-60071
Naphtho[1,8-*bc*]pyran-2-carboxylic acid; Et ester, *in* N-70010

$C_{15}H_{12}O_3S$
2,3-Dihydro-2-phenyl-4*H*-1-benzothiopyran-4-one; 1,1-Dioxide, *in* D-70248
1,4-Dimethylthioxanthone; Dioxide, *in* D-70442
2,4-Dimethylthioxanthone; Dioxide, *in* D-70444
1-(2-Furyl)-4-(5-acetoxymethyl-2-thienyl)-1-buten-3-yne, *in* F-80093
3-Hydroxymethyldibenzo[*b*,*f*]thiepin; 5,5-Dioxide, *in* H-60176
4-[5-(1,3-Pentadiynyl)-7-thienyl]-3-butyn-1-ol; 2-Hydroxy, 1-Ac, *in* P-80025
4-[5-(1,3-Pentadiynyl)-7-thienyl]-3-butyn-1-ol; 2-Hydroxy, 2-Ac, *in* P-80025

$C_{15}H_{12}O_4$
4′,7-Dihydroxyisoflavanone, D-80322
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one, D-80367
3,9-Dihydroxypterocarpan, D-60373
Frutescinone, *in* F-80084
6-Hydroxy-2-(4-hydroxy-2-methoxyphenyl)benzofuran, *in* D-80363
Mycosinol; Ac (*E*-), *in* M-80202
Mycosinol; Ac (*Z*-), *in* M-80202
3-Phenyl-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one, P-80139
2′,4′,7-Trihydroxyisoflavene, T-80305

$C_{15}H_{12}O_5$
4-Acetoxy-8,9-epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-ene, *in* M-80202
3,5-Dihydroxy-2,4-dimethoxy-9*H*-fluoren-9-one, *in* T-70109
1,6-Dihydroxy-5-methoxyxanthone, *in* T-60349
1-(2,4-Dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)-2-propen-1-one, D-80362
1-Hydroxy-3,7-dimethoxyxanthone, *in* T-80347
1-Hydroxy-5,6-dimethoxyxanthone, *in* T-60349
3-(4-Hydroxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, H-80245
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one, H-80246
4-Methoxy-6-(3,4-methylenedioxystyryl)-α-pyrone, *in* M-80086
Protosappanin *A*, P-60186
2′,3′,4′,7-Tetrahydroxyisoflavene, T-80103
2′,4′,7,8-Tetrahydroxyisoflavene, T-80104
4′,5,8-Trihydroxyflavanone, T-80297
5,7,8-Trihydroxyflavanone, T-60321
2′,4′,7-Trihydroxyisoflavanone, T-80303
3′,4′,7-Trihydroxyisoflavanone, T-70263
4′,5,7-Trihydroxyisoflavanone, T-80304
2,3,9-Trihydroxypterocarpan, T-80335
3,4,9-Trihydroxypterocarpan, T-80336
3,9,10-Trihydroxypterocarpan, T-80338
3,6*a*,9-Trihydroxypterocarpan, T-80337

$C_{15}H_{12}O_6$
1,3-Dihydroxy-5,8-dimethoxyxanthone, *in* T-70123
1,8-Dihydroxy-3,5-dimethoxyxanthone, *in* T-70123
1,8-Dihydroxy-3,6-dimethoxyxanthone, *in* T-60127
3,5-Dihydroxy-2-methyl-1,4-naphthoquinone; Di-Ac, *in* D-60350
3-(3,4-Dihydroxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, D-80372
3-(3,4-Dihydroxyphenyl)-1-(2,4,5-trihydroxyphenyl)-2-propen-1-one, D-70339
2′,3′,4′,6,7-Pentahydroxyisoflavene, P-80040
1-(2,3,4,5,6-Pentahydroxyphenyl)-3-phenyl-2-propen-1-one, P-80050
2′,5,7,8-Tetrahydroxyflavanone, T-70104
3′,4′,5,7-Tetrahydroxyflavanone, T-70105
3′,4′,6,7-Tetrahydroxyflavanone, T-70106
3,5,6,7-Tetrahydroxyflavanone, T-60105
2′,3′,4′,7-Tetrahydroxyisoflavanone, T-80099
2′,4′,5,7-Tetrahydroxyisoflavanone, T-80100
2′,4′,5′,7-Tetrahydroxyisoflavanone, T-80101
2,3,8,9-Tetrahydroxypterocarpan, T-80117
2,3,9,10-Tetrahydroxypterocarpan, T-80118
3,4,8,9-Tetrahydroxypterocarpan, T-80119
3,6*a*,7,9-Tetrahydroxypterocarpan, T-80120

$C_{15}H_{12}O_7$
Nectriafurone, N-60016
2′,3,5,7,8-Pentahydroxyflavanone, P-60045
▷ 3,3′,4′,5,7-Pentahydroxyflavanone, P-70027
3′,4′,5,6,7-Pentahydroxyflavanone, P-70028
2′,3′,4′,5,7-Pentahydroxyisoflavanone, P-80039
1,2,3,8,9-Pentahydroxypterocarpan, P-80051
2,3,8,9,10-Pentahydroxypterocarpan, P-80054
3,4,8,9,10-Pentahydroxypterocarpan, P-80055
2,3,6*a*,8,9-Pentahydroxypterocarpan, P-80052
3,4,6*a*,8,9-Pentahydroxypterocarpan, P-80053
3,6*a*,7,8,9-Pentahydroxypterocarpan, P-80056
1,2,5,6,8-Pentahydroxyxanthone, P-60052
1,3,8-Trihydroxy-2,6-dimethoxyxanthone, *in* P-70036
1,5,8-Trihydroxy-2,6-dimethoxyxanthone, *in* P-60052
1,5,10-Trihydroxy-7-methoxy-3-methyl-1*H*-naphtho[2,3-*c*]pyran-6,9-dione, T-80320
Ventilone *C*, V-60004
Ventilone *D*, *in* V-60004

$C_{15}H_{12}O_8$
Fusarubinoic acid, F-70058
2,3,4,8,9,10-Hexahydroxypterocarpan, H-80072

$C_{15}H_{12}O_9$
1-(2,3,4,5-Tetrahydroxyphenyl)-3-(2,4,5-trihydroxyphenyl)-1,3-propanedione, T-70120

$C_{15}H_{12}S$
3-Phenyl-2*H*-1-benzothiopyran, P-80091
4-Phenyl-2*H*-1-benzothiopyran, P-80092

$C_{15}H_{13}Br$
1-Bromo-1,2-diphenylpropene, B-60237
3-Bromo-1,2-diphenylpropene, B-70209

$C_{15}H_{13}ClO$
2,2-Diphenylpropanoic acid; Chloride, *in* D-70493

$C_{15}H_{13}ClO_2$
2-Chloro-3,11-tridecadiene-5,7,9-triyn-1-ol; Ac, *in* C-80117

$C_{15}H_{13}N$
1-Cyano-1,1-diphenylethane, *in* D-70493
10,11-Dihydro-5*H*-dibenzo[*a*,*d*]cyclohepten-5,10-imine, D-80179

$C_{15}H_{13}NO$
N-(Diphenylmethylene)acetamide, *in* D-60482
6-Hydroxyindole; Benzyl ether, *in* H-60158
Phthalimidine; *N*-Benzyl, *in* P-70100

$C_{15}H_{13}NOS$
2-Phenyl-1,5-benzothiazepin-4(5*H*)-one; 2,3-Dihydro, *in* P-60081

$C_{15}H_{13}NO_2$
5-Amino-1,4-pentanediol, A-80132
3,4-Diphenyl-2-oxazolidinone, *in* P-60126

$C_{15}H_{13}NO_2S$
10*H*-Phenothiazine-1-carboxylic acid; *N*-Et, *in* P-70055
10*H*-Phenothiazine-3-carboxylic acid; *N*-Et, *in* P-70057
10*H*-Phenothiazine-4-carboxylic acid; *N*-Et, *in* P-70058
10*H*-Phenothiazine-2-carboxylic acid; Et ester, *in* P-70056
10*H*-Phenothiazine-1-carboxylic acid; *N*-Me, Me ester, *in* P-70055
10*H*-Phenothiazine-2-carboxylic acid; *N*-Me, Me ester, *in* P-70056
10*H*-Phenothiazine-3-carboxylic acid; *N*-Me, Me ester, *in* P-70057
10*H*-Phenothiazine-4-carboxylic acid; *N*-Me, Me ester, *in* P-70058

$C_{15}H_{13}NO_3$
4-Hydroxy-3-methoxy-2-methyl-9*H*-carbazole-1-carboxaldehyde, H-70154

$C_{15}H_{13}NO_4$
Acetaminosalol, *in* H-70108
4-Phenyl-2,6-pyridinedicarboxylic acid; Di-Me ester, *in* P-80130

$C_{15}H_{13}NO_4S$
10*H*-Phenothiazine-3-carboxylic acid; *N*-Et, 5,5-dioxide, *in* P-70057
10*H*-Phenothiazine-4-carboxylic acid; *N*-Me, 5,5-dioxide, Me ester, *in* P-70058
10*H*-Phenothiazine-3-carboxylic acid; *N*-Me, Me ester, 5,5-dioxide, *in* P-70057

$C_{15}H_{13}NO_5$
Dianthramide *A*, D-70049
Dianthramide B, *in* D-70049
1,2,4-Trimethoxy-3*H*-phenoxazin-3-one, T-60353

$C_{15}H_{13}NS_2$
2*H*-1,4-Benzothiazine-3(4*H*)-thione; 4-Benzyl, *in* B-70055

$C_{15}H_{14}$
6,7-Dihydro-5*H*-dibenzo[*a*,*c*]cycloheptene, D-70186

10,11-Dihydro-5*H*-dibenzo[*a*,*d*]cycloheptene, D-60217
1,1-Diphenylcyclopropane, D-60478
1,1-Diphenylpropene, D-60491

$C_{15}H_{14}ClN$
4-Chloro-2,3-dihydro-1*H*-indole; 1-Benzyl, *in* C-60055

$C_{15}H_{14}N_2$
10,11-Dihydro-5*H*-dibenzo[*a*,*d*]cyclohepten-5-one; Hydrazone, *in* D-60218

$C_{15}H_{14}N_2O$
N-(7,7-Dimethyl-3-azabicyclo[4.1.0]hepta-1,3,5-trien-4-yl)benzamide, D-70368

$C_{15}H_{14}N_2OS$
10*H*-Phenothiazine-2-carboxylic acid; Dimethylamide, *in* P-70056

$C_{15}H_{14}N_2O_2$
N,*N*′-Diphenylurea; Mono-*N*-Ac, *in* D-70499

$C_{15}H_{14}N_2S$
2-Amino-4*H*-3,1-benzothiazine; *N*-Benzyl, *in* A-70092

$C_{15}H_{14}N_4$
4-Amino-1,2,3-benzotriazine; 2-Et, *N*(4)-Ph, *in* A-60092
4-Amino-1,2,3-benzotriazine; 3-Et, *N*(4)-Ph, *in* A-60092

$C_{15}H_{14}O$
Di(2,4,6-cycloheptatrien-1-yl)ethanone, D-60166
Linderazulene, L-70031

$C_{15}H_{14}OS$
Thia[2.2]metacyclophane; *S*-Oxide, *in* T-60194

$C_{15}H_{14}O_2$
1-Acetoxy-2,8,10,12-tridecatetraene-4,6-diyne, *in* T-80260
2,2-Diphenylpropanoic acid, D-70493
2-Hydroxy-1,2-diphenyl-1-propanone, H-70123
2-Hydroxy-1,3-diphenyl-1-propanone, H-70124
3-Methoxy-5-(2-phenylethenyl)phenol, *in* D-80384
3,5-Tridecadiene-7,9,11-triyn-1-ol; Ac, *in* T-80258

$C_{15}H_{14}O_2S$
2-Mercapto-2-phenylacetic acid; *S*-Benzyl, *in* M-60024
Thia[2.2]metacyclophane; *S*-Dioxide, *in* T-60194

$C_{15}H_{14}O_2S_2$
3,3-Bis(phenylthio)propanoic acid, B-70157

$C_{15}H_{14}O_3$
4-(Benzyloxy)phenol; Ac, *in* B-60074
Cyclolongipesin, C-60214
Dehydroosthol, D-60020
cis-Dehydroosthol, *in* D-60020
9,10-Dihydro-7-methoxy-2,5-phenanthrenediol, *in* P-80080
Frutescin/, F-80084
4′-Hydroxy-2-biphenylcarboxylic acid; Me ether, Me ester, *in* H-70111

$C_{15}H_{14}O_4$
8-Acetoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-3-ene, *in* H-80047
Allopteroxylin, A-60075
1-(3,5-Dihydroxyphenyl)-2-(3-hydroxy-4-methoxyphenyl)ethylene, *in* D-80361
3-(2,4-Dihydroxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, D-80366
Helicquinone, H-60015
2-Hydroxy-4,6-dimethoxybenzophenone, *in* T-80285
4-Hydroxy-2,6-dimethoxybenzophenone, *in* T-80285
5-[2-(3-Hydroxy-4-methoxyphenyl)ethenyl]-1,3-benzenediol, *in* D-80361
8-(3-Methyl-2-butenoyl)coumarin, *in* M-80190
2-Methyl-1,3-naphthalenediol; Di-Ac, *in* M-60091
4-Methyl-1,3-naphthalenediol; Di-Ac, *in* M-60094
Micropubescin, M-80190
Murralongin, M-70159
Rhinacanthin A, R-80005
Rutalpinin, R-70015
3′,4′,7-Trihydroxyflavan, T-70260
2′,4′,7-Trihydroxyisoflavan, T-80302
1-(2,4,6-Trihydroxyphenyl)-3-phenyl-1-propanone, T-80332
Yangonin, *in* H-70122

$C_{15}H_{14}O_5$
Ageratone, A-60065
Altholactone; Ac, *in* A-60083
Anhydroscandenolide, A-70211
2,3-Dihydro-5-hydroxy-8-methoxy-2,4-dimethylnaphtho[1,2-b]furan-6,9-dione, D-80213
3,6-Dihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]-2,7(1*aH*,7*aH*)-dione, *in* D-70277
6-[2-(4-Hydroxy-3-methoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one, *in* H-70122
1-(4-Hydroxyphenyl)-3-(2,4,6-trihydroxyphenyl)-1-propanone, H-80243
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone, H-80244
Panial, P-70006
3′,4′,5,7-Tetrahydroxyflavan, T-60103
3,4′,5,7-Tetrahydroxyflavanone, T-60104
2′,3′,4′,7-Tetrahydroxyisoflavan, T-80095
2′,4′,5,7-Tetrahydroxyisoflavan, T-80096
2′,4′,5′,7-Tetrahydroxyisoflavan, T-80097
2′,4′,6,7-Tetrahydroxyisoflavan, T-80098

$C_{15}H_{14}O_6$
7-(3,3-Dimethyloxiranyl)methoxy-5,6-methylenedioxycoumarin, D-80463
Fonsecin, F-80073
1,4,5,7-Naphthalenetetrol; 5-Me ether, 1,7-Di-Ac, *in* N-80003
3,3′,4′,5,7-Pentahydroxyflavan, P-70026
2′,3′,4′,7,8-Pentahydroxyisoflavan, P-80038

$C_{15}H_{14}O_7$
Fusarubin, F-60108
2′,3′,4′,6,7,8-Hexahydroxyisoflavan, H-80068
2,5,8-Trihydroxy-3-methyl-6,7-methylenedioxy-1,4-naphthoquinone; Tri-Me ether, *in* T-60333

$C_{15}H_{14}S$
Dimethylsulfonium 9-fluorenylide, D-80475
Thia[2.2]metacyclophane, T-60194

$C_{15}H_{15}N$
10,11-Dihydro-5-methyl-5*H*-dibenz[*b*,*f*]azepine, *in* D-70185
5,6,7,12-Tetrahydrodibenz[*b*,*e*]azocine, T-70055
5,6,11,12-Tetrahydrodibenz[*b*,*f*]azocine, T-70057
5,6,7,12-Tetrahydrodibenz[*b*,*g*]azocine, T-70056
5,6,7,8-Tetrahydrodibenz[*c*,*e*]azocine, T-70054
1,2,3-Trimethyl-9*H*-carbazole, T-60357
1,2,4-Trimethyl-9*H*-carbazole, T-60358
1,3,9-Trimethylcarbazole, *in* D-70375
2,4,9-Trimethylcarbazole, *in* D-70382

$C_{15}H_{15}NO$
2-Acetamido-3-methylbiphenyl, *in* A-70164
4-Amino-3,4-dihydro-2-phenyl-2*H*-1-benzopyran, A-80067
2-Amino-1,3-diphenyl-1-propanone, A-60149
2,2-Diphenylpropanoic acid; Amide, *in* D-70493
1,2,3,4-Tetrahydrobenz[*g*]isoquinoline; *N*-Ac, *in* T-80054

$C_{15}H_{15}NO_2$
2-Hydroxy-1,3-diphenyl-1-propanone; Oxime, *in* H-70124
2-Nitro-1,3-diphenylpropane, N-70048

$C_{15}H_{15}NO_4$
6-Amino-2-hexenoic acid; *N*-Phthalimido, Me ester, *in* A-60173
2,3-Quinolinedicarboxylic acid; Di-Et ester, *in* Q-80002

$C_{15}H_{15}NO_5$
2,3-Quinolinedicarboxylic acid; Di-Et ester, *N*-oxide, *in* Q-80002

$C_{15}H_{15}N_5$
5-Amino-1*H*-tetrazole; 1,5(*N*)-Dibenzyl, *in* A-70202
5-Amino-1*H*-tetrazole; 2,5(*N*)-Dibenzyl, *in* A-70202

$C_{15}H_{16}$
7,8,9,10-Tetrahydro-6*H*-cyclohepta[*b*]naphthalene, T-70047

$C_{15}H_{16}Br_2O_2$
Deoxyokamurallene, D-80030

$C_{15}H_{16}Br_2O_3$
Isookamurallene, I-80067
Okamurallene, O-80028

$C_{15}H_{16}N_2O$
▷ *N*,*N*′-Dimethyl-*N*,*N*′-diphenylurea, *in* D-70499

$C_{15}H_{16}N_4$
2,5-Diphenyl-1,2,4,5-tetraazabicyclo[2.2.1]heptane, D-70498

$C_{15}H_{16}N_{10}O_2$
Drosopterin, D-60521
Isodrosopterin, *in* D-60521
Neodrosopterin, *in* D-60521

$C_{15}H_{16}O$
2,3-Dihydrolinderazulene, *in* L-70031
1,3,5,7(11),9-Guaiapentaen-14-al, G-60039
4-Isopropyl-7-methyl-1-naphthalenecarboxaldehyde, I-80084
8-Isopropyl-5-methyl-2-naphthalenecarboxaldehyde, I-60129
3-Methyl-8-phenyl-3,5,7-octatrien-2-one, M-80144
1,8,10,14-Pentadecatetraene-4,6-diyn-3-ol, P-80022
4-(2-Phenylethyl)phenol; Me ether, *in* P-70073

$C_{15}H_{16}OS_2$
3,3-Bis(phenylthio)-1-propanol, B-70158

$C_{15}H_{16}O_2$
10-Desmethyl-1-methyl-1,3,5(10),11(13)-eudesmatetraen-12,8-olide, D-70026
Furoixiolal, F-70056
3-Methoxy-5-(2-phenylethyl)phenol, *in* P-80100

$C_{15}H_{16}O_2S$
1-Acetoxy-9-(2-thienyl)-4,6-nonadien-8-yne, *in* T-80181

$C_{15}H_{16}O_3$
3-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)-2-propenoic acid; Me ester, *in* D-70372
Gnididione, G-60030
Heritol, H-60028
8-Hydroxy-1(6),2,4,7(11)-cadinatetraen-12,8-olide, H-70114
Hypocretenolide, *in* H-70235
Lumiyomogin, L-70041
2-Oxo-3,10(14),11(13)-guaiatrien-12,6-olide, O-70090
2,3,4-Trimethoxybiphenyl, *in* B-70124
3,4,5-Trimethoxybiphenyl, *in* B-80129
Yomogin, Y-70001

$C_{15}H_{16}O_4$
Auraptenol, A-70269
1,2-Bis(4-hydroxyphenyl)-1,2-propanediol, B-70147
Cedrelopsin, C-60026
1-(2,4-Dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)propane, D-70336
2,6-Dimethoxy-4-(2-methoxyphenyl)phenol, *in* B-80128
3-(1,1-Dimethylallyl)scopoletin, *in* R-80016
3-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, *in* D-80470
2,9-Epoxylactarotropone, E-80038
1α,2α-Epoxyyomogin, *in* Y-70001
Ferreyrantholide, F-70004
8β-Hydroxydehydrozaluzanin *C*, *in* Z-60001
14-Hydroxyhypocretenolide, *in* H-70235

9-Hydroxy-3-oxo-1,4(15),11(13)-eudesmatrien-12,6-olide, H-60202
Isomurralonginol, I-70071
Longipesin, L-60034
6-Methoxy-7-[(3-methyl-2-butenyl)oxy]coumorin, *in* H-80189
Murraol, M-60150
Suberenol, S-70080
5,6,9,10-Tetradehydro-1,4:3,14-diepoxy-4-hydroxy-4,5-secofuranoeremophilane, T-80046

$C_{15}H_{16}O_5$
7-Acetyl-6,8-dihydroxy-3-methoxy-4,4-dimethyl-1(4*H*)-naphthalenone, A-80020
Deoxycollybolidol, *in* C-80147
7,7*a*-Dihydro-3,6,7-trihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]oxiren-2(1*aH*)-one, D-70277
1,4,5,7-Naphthalenetetrol; 1,4,5-Tri-Me ether, Ac, *in* N-80003
Peroxyauraptenol, *in* A-70269
Tenucarb, T-80008

$C_{15}H_{16}O_6$
Collybolidol, C-80147

$C_{15}H_{16}O_7$
Dihydrofusarubin *A*, *in* F-60108
Dihydrofusarubin *B*, *in* F-60108

$C_{15}H_{16}O_8$
5-Methyl-1,2,3,4-benzenetetrol; Tetra-Ac, *in* M-80050
3,4,5-Trihydroxyphenylacetic acid; Tri-Ac, Me ester, *in* T-60343

$C_{15}H_{16}O_9$
Aesculin, *in* D-84287
Cichoriin, *in* D-84287

$C_{15}H_{17}BrN_2O_3$
6-Bromotryptophan; N^{α}-Ac, Et ester, *in* B-60334

$C_{15}H_{17}BrN_2O_7$
5-(2-Bromovinyl)-2′-deoxyuridine; 3′,5′-Di-Ac, *in* B-80266

$C_{15}H_{17}Br_2ClO_3$
Okamurallene chlorohydrin, O-80029

$C_{15}H_{18}$
1-(2,2-Dimethylpropyl)naphthalene, D-60446
2-(2,2-Dimethylpropyl)naphthalene, D-60447
2,3,4,5,6,7,8,9-Octahydro-1*H*-triindene, O-60021

$C_{15}H_{18}Br_2O$
9-Bromolaurenisol, B-80211

$C_{15}H_{18}N_2$
Aurantioclavine, A-60316

$C_{15}H_{18}O$
3,4-Dihydro-8-isopropyl-5-methyl-2-naphthalenecarboxaldehyde, *in* I-60129
8,10,14-Pentadecatriene-4,6-diyn-3-ol, P-80023
Tubipofuran, T-70332

$C_{15}H_{18}O_2$
Alantodiene, A-80042
Isoalantodiene, I-80045
2-Oxoverboccidentafuran, *in* V-70005
Procerin/, P-80175
Secoeurabicanal, S-80012
Secoeurabicol, S-80013
Spiroeuryolide, S-80042
Stevisamolide, S-70073
Tannunolide *A*, T-60005
Tannunolide *B*, *in* T-60005

$C_{15}H_{18}O_3$
6α-Acetoxy-2α-hydroxy-1(10),4,11(13)-germacratrien-12,8-olide, *in* H-70134
Achalensolide, A-70054
Achillin, A-80033
Aquatolide, A-80168
Bullerone, B-60337
11α,13-Dihydroyomogin, *in* Y-70001
Epiligustrin, *in* L-80030
3-Epizaluzanin *C*, *in* Z-60001
Estafiatin, E-80057
7α-Hydroxy-3-deoxyzaluzanin *C*, *in* Z-60001
2-Hydroxy-1,4,6-eudesmatriene-3,8-dione, H-80163
1-Hydroxy-2,4(15),11(13)-eudesmatrien-12,8-olide, H-70129
1-Hydroxy-3,7(11),8-eudesmatrien-12,8-olide, H-60140
1-Hydroxy-4(15),7(11),8-eudesmatrien-12,8-olide, H-60141
8-Hydroxy-4(15),11(13),10(14)-guaiatrien-12,6-olide, H-70138
Inunal, I-70022
Isoinunal, *in* I-70022
Leucomisin, *in* M-80010
Ligustrin, L-80030
Melicophyllone A, M-80012
2-Oxo-1(10),11(13)-eremophiladien-12,8-olide, O-80081
3-Oxo-4,11(13)-eudesmadien-12,8β-olide, *in* H-60136
9-Oxo-4,11(13)-eudesmadien-12,16β-olide, *in* H-60137
1-Oxoisoalantolactone, *in* I-80046
9-Oxoisoalantolactone, *in* I-80046
Zaluzanin *C*, Z-60001
Zederone, Z-70003

$C_{15}H_{18}O_4$
6-Acetyl-7,8-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran, *in* A-80023
Austrisin, *in* M-80010
1,2;3,4-Bisepoxy-11(13)-eudesmen-12,8-olide, B-70142
Carmenin, *in* F-70006
Cooperin, C-70196
8-Deacyl-15-deoxypunctatin, D-80006
8-Desoxyurospermal A, *in* I-80102
Dihydrosuberenol, *in* S-70080
1,5-Dihydroxy-2,4(15),11(13)-eudesmatrien-12,8-olide, D-70298
2,8-Dihydroxy-3,10(14),11(13)-guaiatrien-12,6-olide, D-60327
1β,10β-Epoxyachillin, *in* A-80033
1α,2α-Epoxy-4β,5-dihydroyomogin, *in* Y-70001
10α,14-Epoxyestafiatin, *in* E-80057
10β,14-Epoxyestafiatin, *in* E-80057
1β,10β-Epoxy-8α-hydroxyachillin, *in* H-60100
1,2-Epoxy-3-hydroxy-4,11(13)-eudesmadien-12,8-olide, E-70019
2,6,10-Farnesatriene-1,15;13,9-diolide, F-80001
Ferulidin, F-70006
Grosheimin, G-80042
8-Hydroxyachillin, H-60100
14-Hydroxy-11,13-dihydrohypocretenolide, *in* H-70235
2-Hydroxyligustrin, H-80184
5-Hydroxy-7-methoxy-2-pentyl-4*H*-1-benzopyran-4-one, H-80192
15-Hydroxy-3-oxoalloalantolactone, *in* A-80044
4-Hydroxy-1-oxo-2,11(13)-eudesmadien-12,8-olide, H-70198
8-Hydroxy-3-oxo-1,4,11(13)-eudesmatrien-12-oic acid, H-70199
8α-Hydroxy-2-oxo-4,10(14)-germacradien-12,6α-olide, *in* D-80319
3-Hydroxy-8-oxo-2(9),6-lactaradien-5,13-olide, H-80229
Hypocretenoic acid, H-70235
Melicophyllone B, *in* M-80012
Methyl 4-oxonorpinguisan-12-oate, *in* N-80083
▷ Parthenin, P-80011
Pentalenolactone *E*, P-60055
3-Phenyl-1,1-cyclopentanedicarboxylic acid; Di-Me ester, *in* P-80098

$C_{15}H_{18}O_5$
Artelin, A-60304
Chrysartemin A, C-80127
1,5-Dihydroxy-2-oxo-3,11(13)-eudesmadien-12,8-olide, D-70329
2,9-Dihydroxy-8-oxo-1(10),4,11(13)-germacratrien-12,6-olide, D-60366
2,3-Epoxy-1,4-dihydroxy-7(11),8-eudesmadien-12,8-olide, E-60012
Hieracin *II*, *in* H-80087
2-Hydroxy-12-oxo-4,11(13)-cadinadien-15-oic acid, H-80228
Melicophyllone C, *in* M-80012
Merrillin, M-80034
Secotanapartholide A, S-80018
Secotanapartholide B, *in* S-80018
Tanaparthin peroxide, T-80001

$C_{15}H_{18}O_6$
Araneophthalide, A-60292
Chilenone *B*, C-60034
Obtusinin, *in* H-80189

$C_{15}H_{18}O_8$
Neoliacinic acid, N-70026

$C_{15}H_{18}O_9$
5,7-Dihydroxy-1(3*H*)-isobenzofuranone; 5-Me ether, glucoside, *in* D-60339
Isolespedezic acid, *in* L-80024
Lespedezic acid, L-80024

$C_{15}H_{19}Br$
1-[3-(Bromomethyl)-1-methyl-2-methylenecyclopentyl]-4-methylbenzene, *in* B-70247

$C_{15}H_{19}ClO_5$
Andalucin, A-70207

$C_{15}H_{19}NO_4$
Pinthuamide, P-80151

$C_{15}H_{19}NO_{10}$
2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one; *O*-β-D-Glucoside, *in* D-10388

$C_{15}H_{19}N_5O_5$
3,4-Dihydro-4,6,7-trimethyl-3-β-D-ribofuranosyl-9*H*-imidazo[1,2-*a*]purin-9-one, D-60302

$C_{15}H_{20}BrClO_2$
Epoxyisodihydrorhodophytin, E-60024

$C_{15}H_{20}Br_2O_2$
Dehydrochloroprepacifenol, D-60018
Isolaureatin, I-70067

$C_{15}H_{20}O$
Dehydrocurcuphenol, *in* C-70208
Dehydrodendrolasin, D-80022
Dehydrodendrolasin; 5*Z*-Isomer, *in* D-80022
Herbacin, H-60027
Parvifoline, P-80013
Periplanone D_1, P-80069
Primnatrienone, P-80174
Verboccidentafuran, V-70005

$C_{15}H_{20}OS$
Thiofurodysin, T-70178
Thiofurodysinin, T-70179

$C_{15}H_{20}O_2$
Alloalantolactone, A-80044
Aristolactone, A-60296
4,6,11(13)-Cadinatrien-12-oic acid, *in* C-70004
Cantabradienic acid, C-60009
6-Deoxyilludin *M*, *in* I-60001
Elemasteiractinolide, E-70005
8,12-Epoxy-3,7,11-eudesmatrien-1-ol, E-60020
1(10),4,11(13)-Germacratrien-8,12-olide, G-70010
Glechomanolide, G-60022
1(10),3-Guaiadien-12,8-olide, G-70032
4,11(13)-Guaiadien-12,8β-olide, *in* A-70054
6-Hydroxyprimnatrienone, *in* P-80174
Isoalantolactone, I-80046
Isoalloalantolactone, I-80047
Isomyomontanone, *in* M-60155
Mansonone A, M-80006
Mokkolactone, M-60142
Myomontanone, M-60155
Nardonoxide, N-70018
Pallescensone, P-70003
Pinguisanin, P-60155
Pulicaral, P-80190
Verboccidentafuran 4α,5α-epoxide, *in* V-70005

$C_{15}H_{20}O_3$
Arteannuin *B*, A-70262
Artemorin, A-80170
Artesovin, A-60306
4,8-Bis-*epi-inuviscolide*, *in* I-70023

Bisabolangelone, B-60138
Cantabrenonic acid, *in* C-60010
Carpesialactone, C-80027
Cumambranolide, C-80164
Cyclodehydromyopyrone *A*, C-60188
Cyclodehydromyopyrone *B*, C-60189
Dehydromyoporone, D-60019
6-Deoxyilludin *S*, *in* I-60002
Desacetyllaurenobiolide, *in* H-70134
11α,13-Dihydroestafialin, *in* E-80057
11α,13-Dihydrozaluzanin *C*, *in* Z-60001
11β,13-Dihydrozaluzanin *C*, *in* Z-60001
Elemasteiractinolide; 15-Hydroxy, *in* E-70005
10-Epicumambranolide, *in* C-80164
1,10-Epoxy-11(13)-eremophilen-12,8-olide, E-80024
1,10-Epoxy-4,11(13)-germacradien-12,8-olide, E-60022
4α,15-Epoxyisoalantolactone, *in* I-80046
9,11(13)-Eremophiladien-12-oic acid; 3-Oxo, *in* E-70029
3,11(13)-Eudesmadien-12-oic acid; 2-Oxo, *in* E-70060
Eumorphistonol, E-60073
Haageanolide, H-60001
Hanphyllin, H-60006
10-Hydroxy-1,11(13)-eremophiladien-12,8-olide, H-80159
15-Hydroxy-4,11(13)-eudesmadien-12,8-olide, H-60138
2-Hydroxy-3,11(13)-eudesmadien-12,8-olide, H-80161
3-Hydroxy-4,11(13)-eudesmadien-12,8-olide, H-60136
7-Hydroxy-4,11(13)-eudesmadien-12,6-olide, H-70128
7-Hydroxy-4,11(13)-eudesmadien-12,6-olide, H-80162
9-Hydroxy-4,11(13)-eudesmadien-12,6-olide, H-60137
3-Hydroxy-1,4(15),11(13)-eudesmatrien-12-oic acid, H-80164
6-Hydroxy-1(10),4,11(13)-germacratrien-12,8-olide, H-70134
15-Hydroxy-3,10(14)-guaiadien-12,8-olide, H-70136
3-Hydroxy-4,11(13)-guaiadien-12,8-olide, H-70135
4-Hydroxy-1(10),11(13)-guaiadien-12,8-olide, H-80167
5-Hydroxy-3,11(13)-guaiatrien-12,8-olide, H-70137
9α-Hydroxyisoalantolactone, *in* I-80046
9β-Hydroxyisoalantolactone, *in* I-80046
15-Hydroxyisoalloalantolactone, *in* I-80047
▷ Illudin *M*, I-60001
Inunal; Δ^4-Isomer, 15-alcohol, *in* I-70022
Inuviscolide, I-70023
Isoperezone, I-70075
Ivangustin, I-70109
Kanshone *C*, K-70006
Muzigadial, M-80201
3-Oxo-4,11(13)-eudesmadien-12-oic acid, *in* E-70061
9-Oxo-4,11(13)-eudesmadien-12-oic acid, *in* H-60135
1-Oxo-7(11)-eudesmen-12,8-olide, O-60067
1-Oxo-4,10(14)-germacradien-12,6α-olide, *in* O-60068
α-Pipitzol, P-60158
Pulicaric acid, *in* P-80190
Quadrangolide, Q-60001
Santamarine, S-60007
Subergorgic acid, S-70081

$C_{15}H_{20}O_4$
Artecalin, A-60302
Confertin, *in* D-60211
Cumambrin B, *in* C-80164
2,3-Dehydro-11α,13-dihydroconfertin, *in* D-60211
11,13-Dehydroeriolin, *in* E-60036
Dehydromelitensin, *in* M-80013
11β,13-Dihydro-9α-hydroxyzaluzanin *C*, *in* Z-60001
Dihydroparthenin, *in* P-80011
3α,15-Dihydroxyalloalantolactone, *in* A-80044
1,8-Dihydroxy-3,7(11)-eremophiladien-12,8-olide, D-60320
1,5-Dihydroxyeriocephaloide, D-60321
1,8-Dihydroxy-3,7(11)-eudesmadien-12,8-olide, D-60322
1,8-Dihydroxy-4(15),11(13)-eudesmadien-12,6-olide, D-80315
2,8-Dihydroxy-4,10(14)-germacradien-12,6-olide, D-80319
2,8-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, D-70302
3,13-Dihydroxy-1(10),4,7(11)-germacratrien-12,6-olide, D-70303
8,9-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, D-60323
9,15-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, D-60324
2,4-Dihydroxy-5,11(13)-guaiadien-12,8-olide, D-70304
3,5-Dihydroxy-4(15),10(14)-guaiadien-12,8-olide, D-60325
4,10-Dihydroxy-2,11(13)-guaiadien-12,6-olide, D-60326
3β,9β-Dihydroxy-4(15),10(14)-guaiadien-12,6α-olide, *in* D-70305
9,10-Dihydroxy-7-marasmen-5,13-olide, D-60346
4,5-Dioxo-1(10)-xanthen-12,8-olide, D-60474
4-Epivulgarin, *in* V-80013
Epoxycantabronic acid, *in* C-60010
1β,10α-Epoxyhaageanolide, *in* H-60001
1,10-Epoxy-13-hydroxy-7(11)-eremophilen-12,8-olide, E-80031
1α,2α-Epoxy-10α-hydroxy-11(13)-eremophilen-12,8β-olide, *in* H-80159
1β,10β-Epoxy-2α-hydroxy-11(13)-eremophilen-12,8β-olide, *in* E-80024
4α,5α-Epoxy-3α-hydroxy-11(13)-eudesmen-12,8β-olide, *in* H-60136
4α,5α-Epoxy-3β-hydroxy-11(13)-eudesmen-12,8β-olide, *in* H-60136
4α,15-Epoxy-3α-hydroxyisoalantolactone, *in* I-80046
4α,13-Epoxymuzigadial, *in* M-80201
Grosheiminol, *in* G-80042
3α-Hydroperoxy-4,11(13)-eudesmadien-12,8β-olide, *in* H-60136
2α-Hydroxyartemorin, *in* A-80170
9β-Hydroxyartemorin, *in* A-80170
8α-Hydroxybalchanin, *in* S-60007
8α-Hydroxy-11α,13-dihydrozaluzanin *C*, *in* Z-60001
6α-Hydroxy-8-epiivangustin, *in* I-70109
6-(1-Hydroxyethyl)-7,8-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran, *in* A-80023
2α-Hydroxyivangustin, *in* I-70109
1-[2-(Hydroxymethyl)-3-methoxyphenyl]-1,5-heptadiene-3,4-diol, H-70178
9β-Hydroxy-3-oxo-10(14)-guaien-12,6α-olide, *in* D-70305
9α-Hydroxysantamarine, *in* S-60007
▷ Illudin *S*, I-60002
Ivangulic acid, I-70108
Ixerin A, I-80102
Kanshone E, *in* K-80003
Pulverulide, P-80191
Ridentin, R-70007
Schkuhridin *B*, S-60012
8,9,14-Trihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, T-60323
Umbellifolide, U-60001
▷ Vulgarin, V-80013

$C_{15}H_{20}O_5$
Alhanin, *in* I-70066
Altamisic acid, A-70084
▷ Coriolin, C-70199
3,5-Dihydroxy-4(15),10(14)-guaiadien-12,8-olide; 10α,14-Epoxide, *in* D-60325
4,5-Epoxy-2,8-dihydroxy-1(10),11(13)-germacradien-12,6-olide, E-60013
Hieracin I, H-80087
Hirsutinolide, H-80089
4α-Hydroperoxydesoxyvulgarin, *in* V-80013
7′-Hydroxyabscisic acid, H-70098
8′-Hydroxyabscisic acid, H-70099
Psilostachyin, P-70131
Secoisoerivanin pseudoacid, S-70024
1,3,13-Trihydroxy-4(15),7(11)-eudesmadien-12,6-olide, T-70258
1,3,9-Trihydroxy-4(15),11(13)-eudesmadien-12,6-olide, T-70257
1β,3α,6β-Trihydroxy-4,11(13)-eudesmadien-12,8β-olide, *in* I-70109

$C_{15}H_{20}O_6$
Ajafinin, A-60068
2,3-Epoxy-1,4,8-trihydroxy-7(11)-eudesmen-12,8-olide, E-60033

$C_{15}H_{20}O_7$
8-Deacyltrichogoniolide, D-80007
Domesticoside, *in* T-70248
Neomajucin, *in* M-70005

$C_{15}H_{20}O_8$
▷ Anisatin, A-80158
Majucin, M-70005
Laurencia Polyketal, P-60168

$C_{15}H_{20}O_{10}$
Quinic acid; Tetra-Ac, *in* Q-70005

$C_{15}H_{21}Br$
1-[3-(Bromomethyl)-1-methyl-2-methylenecyclopentyl]-4-methyl-1,4-cyclohexadiene, B-70247

$C_{15}H_{21}BrO$
Isoobtusadiene, I-70074
Obtusadiene, O-70001

$C_{15}H_{21}BrO_3$
Laureoxolane, L-80022

$C_{15}H_{21}Br_3O_3$
Intricata bromoallene, I-80016
3,6,13-Tribromo-4,10:9,12-diepoxy-14-pentadecyn-7-ol, B-70195

$C_{15}H_{21}ClO$
Laurencenone *B*, L-70025

$C_{15}H_{21}ClO_3$
10α-Chloro-1β-hydroxy-11(13)-eremophilen-12,8β-olide, *in* D-80314

$C_{15}H_{21}NO$
Octahydro-2*H*-1,3-benzoxazine; *N*-Benzyl, *in* O-70011
Octahydro-2*H*-3,1-benzoxazine; *N*-Benzyl, *in* O-70012

$C_{15}H_{21}NO_4$
3,5-Pyridinedipropanoic acid; Di-Et ester, *in* P-60217

$C_{15}H_{21}N_3O_3$
3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]oxazine; Tri-*N*-Me, *in* H-80054

$C_{15}H_{21}N_3S_3$
3,4,7,8,11,12-Hexahydro-2*H*,6*H*,10*H*-benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1,4]thiazine; Tri-*N*-Me, *in* H-80055

$C_{15}H_{22}$
1(10),4-Aromadendradiene, A-70257
1(5),3-Aromadendradiene, A-70256
1,1,2,2,3,3-Hexamethylindane, H-80075

$C_{15}H_{22}BrClO$
Elatol, E-70002
Laurencenone *A*, L-70024
Laurencenone *D*, L-70026

$C_{15}H_{22}BrClO_2$
Almadioxide, A-80047
Pinnatazone, P-80150

$C_{15}H_{22}Br_2O_3$
α-(1-Bromo-3-hexenyl)-5-(1-bromo-2-propynyl)tetrahydro-3-hydroxy-2-furanethanol, B-70217

$C_{15}H_{22}N_2O_4$
N-(5*a*,6,7,8-Tetrahydro-4-methyl-1,5-dioxo-1*H*,5*H*-pyrrolo[1,2-*c*][1,3]oxazepin-3-yl)hexanamide, *in* M-70134

$C_{15}H_{22}O$
1(10)-Aristolen-9-one, A-70252
13-Bicyclogermacrenal, B-80076
1,9-Cadinadien-3-one, C-80003
2-Copaen-8-one, C-80149

Curcuphenol, C-70208
Cyperenal, *in* C-70259
Elvirol, E-60004
11,12-Epoxy-10(14)-guaien-4-ol, E-80028
4,11-Eudesmadien-3-one, E-80081
Grimaldone, G-70030
4,11(13)-Guaiadien-3-one, G-80043
4,11-Guaiadien-3-one, G-80044
Isobicyclogermacrenal, I-60088
Laurencenone *C*, *in* L-70025
Nuciferol, N-70082
Penlanpallescensin, P-60015
6,8,10,12-Pentadecatetraenal, P-80021
Perforenone, P-60063
Periplanone D_2, *in* P-80069
Premnaspiral, *in* P-70114
12-Sesquisabinenal, *in* S-70037
3-Silphinenone, S-60033
Solavetivone, S-70051
Tochuinol, T-70202
Xanthorrhizol, X-70001

$C_{15}H_{22}O_2$
Aglycone A_3, *in* S-70051
Anhydroarthrosporone, A-80157
Apotrisporin *C*, *in* A-70247
1(10),4-Bicyclogermacradien-13-oic acid, B-80075
4,11(13)-Cadinadien-12-oic acid, C-70004
Capsenone, C-60011
Cinnamolide, C-80133
Cyparenoic acid, C-70258
Dihydroisoalantolactone, *in* I-80046
Drimenin, D-60519
10,11-Epoxy-2,7(14)-bisaboladien-4-one, E-80014
4,5-Epoxy-1(10),7(11)-germacradien-8-one, E-60023
9,11(13)-Eremophiladien-12-oic acid, E-70029
▷ 3,11(13)-Eudesmadien-12-oic acid, E-70060
4,11(13)-Eudesmadien-12-oic acid, E-70061
4-Guaien-12,8β-olide, *in* A-70054
Helminthosporal, H-60016
HM-1, H-80091
HM-4, H-80094
6-Hydroxy-2,7,10-bisabolatrien-9-one, H-60107
4-Hydroxy-1,9-cadinadien-3-one, H-80136
2-Hydroxy-4,11(13)-eudesmadien-15-al, H-80160
2-Hydroxy-4,11(13)-eudesmadien-15-al; 2α-*form*, *in* H-80160
6-Hydroxy-1,4-eudesmadien-3-one, H-60139
12-Hydroxy-4,11(13)-eudesmadien-3-one, *in* E-80081
Kanshone *A*, K-70004
Mandassidione, M-80004
2-Oxoisoanhydrooplopanone, *in* O-50045
10-Oxo-6-isodaucen-14-al, O-70093
Oxysolavetivone, *in* S-70051
9-Phenylnonanoic acid, P-70084

$C_{15}H_{22}O_3$
Apotrisporin *E*, A-70247
Artausin, A-70261
Artedouglasiaoxide, A-70263
Bedfordiolide, B-60008
Brassicadiol, B-70177
Cantabrenolic acid, C-60010
2-Deoxy-4-epipulchellin, *in* P-80189
11β,13-Dihydro-8-*epi-confertin*, *in* D-60211
11β,13-Dihydro-1-*epi-inuviscolide*, *in* I-70023
Dihydroconfertin, D-60211
11β,13-Dihydroconfertin, *in* D-60211
11α,13-Dihydroinuviscolide, *in* I-70023
11β,13-Dihydroinuviscolide, *in* I-70023
Dihydroparthenolide, D-70239
12,13-Dihydroxy-1(10)-aromadendren-2-one, D-70283
3,8-Dihydroxylactariusfuran, D-70312
4,8-Dihydroxylactariusfuran, D-70313
7,13-Dihydroxy-2-longipinen-1-one, D-70315
7,9-Dihydroxy-2-longipinen-1-one, D-80332
8β,9α-Dihydroxy-4,10(14)-oplopadien-3-one, *in* O-70042
3-(1,3,5,7,9-Dodecapentaenyloxy)-1,2-propanediol, D-70536
Elemasteiractinolide; 11β,13-Dihydro, 15-hydroxy, *in* E-70005
11,13-Epoxy-4-cadinen-15-oic acid, *in* H-80135
1,10-Epoxy-11(13)-eremophilen-12-oic acid, E-80023
1β,10β-Epoxy-11α*H*-eremophilen-12,8β-olide, *in* E-80024
3,4-Epoxy-11(13)-eudesmen-12-oic acid, E-60021
12,13-Epoxytrichothec-9-en-3-ol, E-70028
9,11(13)-Eremophiladien-12-oic acid; 2β-Hydroxy, *in* E-70029
9,11(13)-Eremophiladien-12-oic acid; 3β-Hydroxy, *in* E-70029
3,11(13)-Eudesmadien-12-oic acid; 2α-Hydroxy, *in* E-70060
4,11(13)-Eudesmadien-12-oic acid; 3β-Hydroxy, *in* E-70061
Furanoeremophilane-2,9-diol, F-70047
10-Hydroxy-2,7(14),11-bisabolatrien-4-one, H-80132
12-Hydroxy-4,11(13)-cadinadien-15-oic acid, H-80135
12-Hydroxy-4,11(13)-cadinadien-15-oic acid; 6,7-Diepimer, *in* H-80135
9α-Hydroxycinnamolide, *in* C-80133
3β-Hydroxy-11β,13-dihydrodesoxoachalensolide, *in* H-70135
9-Hydroxy-4,11(13)-eudesmadien-12-oic acid, H-60135
2-Hydroxy-5-eudesmen-12,8-olide, H-80165
3-Hydroxy-4-eudesmen-12,8-olide, H-80166
4-Hydroxy-11(13)-eudesmen-12,8-olide, H-60142
4-Hydroxy-10(14)-guaien-12,8-olide, H-80168
4-Hydroxy-9-guaien-12,8-olide, H-80169
Ketosantalic acid, K-70012
Myoporone, M-60156
9-Oxo-2,7-bisaboladien-15-oic acid, O-80066
1-Oxo-4-germacren-12,6-olide, O-60068
7-Oxo-11-nordrim-8-en-12-oic acid; Me ester, *in* O-60080
Oxycurcumenol, O-80101
Pentalenic acid, P-60054
Piperdial, P-80152
Sambucoin, S-70007
Santamarine; 11β,13-Dihydro, *in* S-60007
Shonachalin *D*, S-70040
Sterpuric acid, S-60053
Temisin, T-80006
Warburganal, W-60001

$C_{15}H_{22}O_4$
Alhanol, I-70066
Artapshin, A-60301
Avenaciolide, A-60325
Cyperanic acid, C-80203
Desacylligulatin *C*, D-70025
Dihydroiresone, *in* I-80043
Dihydroridentin, *in* R-70007
1,10-Dihydroxy-11(13)-eremophilen-12,8-olide, D-80314
1,3-Dihydroxy-4-eudesmen-12,6-olide, D-70299
1,8-Dihydroxy-4(15)-eudesmen-12,6-olide, D-80316
2α,11α-Dihydroxy-5-eudesmen-12,8β-olide, *in* H-80165
1β,3α-Dihydroxy-4-eudesmen-12,6α-olide, *in* I-70066
1,3-Dihydroxy-4,10(14)-germacradien-12,6-olide, D-80317
1,3-Dihydroxy-4,9-germacradien-12,6-olide, D-80318
8,14-Dihydroxy-1(10),4-germacradien-12,6-olide, D-80320
3,9-Dihydroxy-10(14)-guaien-12,6-olide, D-70305
8,10-Dihydroxy-3-guaien-12,6-olide, D-60328
11-Epidihydroridentin, *in* R-70007
1-Epierivanin, *in* E-70033
4-Epineopulchellin, *in* N-70028
1β,10β-Epoxy-2α-hydroxy-11α*H*-eremophilen-12,8β-olide, *in* E-80024
1β,10β-Epoxy-2α-hydroxy-11β*H*-eremophilen-12,8β-olide, *in* E-80024
1β,10β-Epoxy-3α-hydroxy-11β*H*-eremophilen-12,8β-olide, *in* E-80024
Eriolin, E-60036
Erivanin, E-70033
Gallicadiol, G-70001
Grangolide, G-80036
11β-Hydroxy-11,13-dihydro-8-*epi-confertin*, *in* D-60211
2α-Hydroxydihydroparthenolide, *in* D-70239
9α-Hydroxydihydroparthenolide, *in* D-70239
9α-Hydroxy-11β,13-dihyrosantamarine, *in* S-60007
8α-Hydroxysambucoin, *in* S-70007
8β-Hydroxysambucoin, *in* S-70007
13-Hydroxysterpuric acid, *in* S-60053
Iresin, I-80043
Isoiresin, *in* I-80043
Ixerin K, *in* I-80102
Ixerin L, *in* I-80102
Kanshone *B*, K-70005
Kanshone D, K-80003
Lactarorufin *D*, L-70016
Lactarorufin *E*, *in* L-70016
Melitensin, M-80013
Neopulchellin, N-70028
Pulchellin A, P-80189
Rugosal A, R-80015
4,5-Seconeopulchell-5-ene, S-70025
Sporol, S-70069
Zafronic acid, Z-70001

$C_{15}H_{22}O_4S$
2*H*-Thiopyran-2,2-dicarboxylic acid; Di-*tert*-butyl ester, *in* T-80191

$C_{15}H_{22}O_5$
11,13-Dihydropsilostachyin, *in* P-70131
9β,10β-Epoxy-1α,3β-dihydroxy-4*Z*-germacren-12,6α-olide, *in* D-80318
2α-Hydroxy-11α,13-dihydroconfertin, *in* D-60211
6α-Hydroxypulchellin, *in* P-80189
4-Oxo-3,4-secoambrosan-12,6-olid-3-oic acid, O-60093
1,4,6-Trihydroxy-11(13)-eudesmen-12,8-olide, T-70259

$C_{15}H_{22}O_6$
3,4,8,10-Tetrahydroxy-1-guaien-12,6-olide, T-80094

$C_{15}H_{22}O_9$
Aucubin, *in* A-80186
6-Deoxycatalpol, *in* C-70026
6-Epiaucubin, *in* A-80186
Eranthemoside, E-60034
Galiridoside, G-60002

$C_{15}H_{22}O_{10}$
Catalpol, C-70026
6-Epimonomelittoside, *in* M-70019
Monomelittoside, *in* M-70019

$C_{15}H_{23}Br$
10-Bromo-2,7-chamigradiene, B-80184

$C_{15}H_{23}Br_2ClO$
2,10-Dibromo-3-chloro-7-chamigren-9-ol, D-80081
Laucopyranoid A, L-80020

$C_{15}H_{23}Br_2ClO_2$
4,10-Dibromo-3-chloro-7,8-epoxy-9-hydroxy-α-chamigrane, D-80083
Laucopyranoid B, L-80021
Laucopyranoid C, *in* L-80021

$C_{15}H_{23}ClO$
4-Chloro-9*R-hydroxy*-3,7(14)-*chamigradiene*, *in* E-70002

$C_{15}H_{23}ClO_2$
2-Chloro-3,7-epoxy-9-chamigranone, C-60066
2-Chloro-3-hydroxy-7-chamigren-9-one, C-60094

$C_{15}H_{23}N$
[10](2,6)Pyridinophane, P-80215

$C_{15}H_{23}NO$
2-Octylamine; *N*-Benzoyl, *in* O-60031
[10](2,6)Pyridinophane; *N*-Oxide, *in* P-80215

$C_{15}H_{23}NO_3$
Parthenolidine, P-80012

$C_{15}H_{24}$
Agarospirene, *in* P-70114

1-Aromadendrene, A-70258
9-Aromadendrene, A-70259
β-Bisabolene, B-80134
4(15),5-Cadinadiene, C-70003
ε-Cadinene, C-60001
Daucene, D-70008
1,3,7(11)-Elematriene, E-70006
1-Epi-α-gurjunene, *in* G-70034
1(5),6-Guaiadiene, G-70031
α-Gurjunene, G-70034
1,1,3,3,5,5-Hexamethyl-2,4,6-tris(methylene)cyclohexane, H-60072
Hinesene, H-80088
1,2,3,4,4*a*,5,6,7-Octahydro-4*a*,5-dimethyl-2-(1-methylethenyl)naphthalene, O-60015
β-Patchoulene, P-60010
Pentalenene, P-70037
Precapnelladiene, P-60171
Premnaspirodiene, P-70114
Sesquisabinene, S-70037
Sesquithujene, *in* S-70037
6-Siliphiperfolene, S-70043
Sinularene, S-60034

$C_{15}H_{24}BrClO$
Puertitol A, P-80187
Puertitol B, P-80188

$C_{15}H_{24}O$
1(5)-Aromadendren-7-ol, A-70260
α-Biotol, B-60112
β-Biotol, B-60113
α-Copaene, C-70197
15-Copaenol, *in* C-70197
α-Copaen-11-ol, *in* C-70197
α-Copaen-8-ol, *in* C-70197
Cyperenol, C-70259
2,3-Epoxy-7,10-bisaboladiene, E-60009
3,5-Eudesmadien-1-ol, E-60064
5,7(11)-Eudesmadien-15-ol, E-60066
5,7-Eudesmadien-11-ol, E-60065
Fervanol, F-60007
1(10),4(15)-Germacradien-6-one, G-80011
Gymnomitrol, G-70035
Jasionone, J-80003
4,10(14)-Oplopadien-3-ol, O-80046
Oplopenone, O-50045
Senecrassidiol; 6α-Hydroxy, 6,8-dideoxy, 7,8-didehydro, *in* S-80026
Sesquisabinene hydrate, *in* S-70037
5-Silphiperfolen-3-ol, S-80033
3-Sterpurenol, S-80045
Striatenone, S-80046
α-Torosol, T-60225
β-Torosol, T-60226
Valerenol, V-70001
Waitziacuminone, W-80001

$C_{15}H_{24}O_2$
10(14)-Aromadendrene-4,8-diol, A-60299
Artemone, A-60305
1(10),4-Cadinadiene-3,9-diol, C-80001
Curcudiol, C-70207
cis-9,10-Dihydrocapsenone, *in* C-60011
10,11-Dihydro-11-hydroxycurcuphenol, *in* C-70208
7,12-Dihydroxysterpurene, D-70346
9,12-Dihydroxysterpurene, D-70347
1,3,11-Elematriene-9,14-diol, E-80010
4,7(11)-Eudesmadiene-12,13-diol, E-60063
11-Hydroxy-2,7(14)-bisaboladien-4-one, H-80131
11-Hydroxy-4-guaien-3-one, H-60149
10α-Hydroxy-6-isodaucen-14-al, *in* O-70093
11-Hydroxyjasionone, *in* J-80003
4-Hydroxy-10(15)-oplopen-3-one, H-80225
11-Hydroxy-1(10)-valencen-2-one, H-60234
Kurubasch aldehyde, K-60014
6-Oxocyclonerolidol, *in* H-60111
Senecrassidiol; 5-Deoxy, 6-oxo, *in* S-80026
Tanavulgarol, T-60004
3,7,11-Trimethyl-2,6,10-dodecatrienoic acid, T-60364
Vetidiol, V-60007

$C_{15}H_{24}O_3$
Arthrosporone, *in* A-80171
Dihydromyoporone, *in* M-60156
3,11-Dihydroxy-7-drimen-6-one, D-70295
8α,9α-Dihydroxy-10β*H*-eremophil-11-en-2-one, *in* E-70030
1,4-Dimethyl-4-[4-hydroxy-2-(hydroxymethyl)-1-methyl-2-cyclopentenyl]-2-cyclohexen-1-ol, D-70417
Feruone, F-70007
FS-2, F-60078
12-Hydroxy-4-cadinen-15-oic acid, *in* H-80135
Isolancifolide, *in* L-80017
Lancifolide, L-80017
Lapidol, L-60014
4,10(14)-Muuroladiene-1,3,9-triol, M-80200
4,10(14)-Oplopadiene-3,8,9-triol, O-70042
9-Oxo-2-bisabolen-15-oic acid, *in* O-80066
Piperalol, *in* P-80152
Punctaporonin *A*, P-60197
Punctaporonin *D*, *in* P-60197
Urodiolenone, U-70006
Zedoarondiol, Z-70004

$C_{15}H_{24}O_4$
Dendroserin, D-80028
Dihydroiresin, *in* I-80043
1β,10α-Dihydroxy-11β*H*-eremophilan-12,8β-olide, *in* D-80314
4-Epipulchellin, *in* P-80189
Secofloribundione, S-70022
Trichotriol, T-60258
5,8,9-Trihydroxy-10(14)-oplopen-3-one, T-70272
Vestic acid, V-70008

$C_{15}H_{24}O_5$
Odontin, O-80027
Rudbeckin *A*, R-70013
1,3,4-Trihydroxy-12,6-eudesmanolide, T-80296

$C_{15}H_{24}O_{11}$
Avicennioside, A-60326

$C_{15}H_{25}BrO$
Brasudol, B-60197
Isobrasudol, *in* B-60197

$C_{15}H_{25}Br_2ClO$
Caespitane, *in* C-80005

$C_{15}H_{25}Br_2ClO_2$
Caespitol, C-80005

$C_{15}H_{25}Br_2ClO_3$
6-Hydroxycaespitol, *in* C-80005

$C_{15}H_{25}NS$
6-Isothiocyano-4(15)-eudesmene, *in* F-60069

$C_{15}H_{26}$
Cyclopentadecyne, C-60220

$C_{15}H_{26}O$
4-Ambiguen-1-ol, A-80056
β-Caryophyllene alcohol, C-80028
Cerapicol, C-70032
Ceratopicanol, C-70033
9(11)-Drimen-8-ol, D-60520
7-Epi-α-eudesmol, *in* E-80086
5,8-Epoxydaucane, E-80021
1(10)-Eremophilen-7-ol, E-70031
11-Eudesmen-5-ol, E-60069
3-Eudesmen-11-ol, E-80086
3-Eudesmen-6-ol, E-70065
4(15)-Eudesmen-11-ol, E-70066
6-Eudesmen-4-ol, E-80087
7-Isopropyl-2,10-dimethylspiro[4.5]dec-1-en-6-ol, I-80079
Naviculol, N-80017
Panasinsanol *A*, P-70005
Panasinsanol *B*, *in* P-70005
2,4-Pentadecadienal, P-70024
Valerenenol, V-80001

$C_{15}H_{26}O_2$
Alloaromadendrane-4,10-diol, A-60074
1,10-Bisaboladiene-3,6-diol, B-80132
3,10-Bisaboladiene-7,14-diol, B-80133
8-Daucene-5,7-diol, D-80004
Debneyol, D-70010
Decahydro-5,5,8*a*-trimethyl-2-naphthalenol; Ac, *in* D-70014
7-Epidebneyol, *in* D-70010
1,4-Epoxy-6-eudesmanol, E-60019
1,4-Epoxy-6-eudesmanol, E-80026
11-Eudesmene-1,5-diol, E-60067
3-Eudesmene-1,6-diol, E-80083
4(15)-Eudesmene-1,11-diol, E-70064
4(15)-Eudesmene-1,6-diol, E-80084
4(15)-Eudesmene-2,11-diol, E-80085
Fauronol, F-70002
1(10),4-Germacradiene-6,8-diol, G-60014
1(10),5-Germacradiene-3,4-diol, G-80010
5,10(14)-Germacradiene-1,4-diol, G-70009
6-Hydroxycyclonerolidol, H-60111
Jaeschkeanadiol, J-70001
Oplopanone, O-70043
Senecrassidiol, S-80026
2,6,10-Trimethyl-2,6,11-dodecatriene-1,10-diol, T-70283
3,7,11-Trimethyl-1,6,10-dodecatriene-3,9-diol, T-70284

$C_{15}H_{26}O_3$
Arthrosporol, A-80171
8-Carotene-4,6,10-triol, C-60021
Caucalol, C-80029
8(14)-Daucene-4,6,9-triol, D-60005
8-Daucene-3,6,14-triol, D-60004
1-*O*-(4,6,8-Dodecatrienyl)glycerol, D-80526
6-Drimene-8,9,11-triol, D-70547
7-Drimene-6,9,11-triol, D-70548
8-Epipertriol, *in* P-80152
6,15-Epoxy-1,4-eudesmanediol, E-80025
11-Eremophilene-2,8,9-triol, E-70030
4(15)-Eudesmene-1,5,6-triol, E-60068
Fexerol, F-60009
5-Hydroperoxy-4(15)-eudesmen-11-ol, H-70097
1-Hydroxydebneyol, *in* D-70010
8-Hydroxydebneyol, *in* D-70010
Shiromodiol, S-70039

$C_{15}H_{26}O_4$
8-Daucene-2,4,6,10-tetrol, D-70009
7,8-Epoxy-4,6,9-daucanetriol, E-80022
Fercoperol, F-60001
3-Hydroperoxy-4-eudesmene-1,6-diol, H-80101
4-Hydroperoxy-2-eudesmene-1,6-diol, H-80102
3-Hydroxymethyl-7,11-dimethyl-2,6,11-dodecatriene-1,5,10-triol, H-70174
2,6,10-Trimethyl-2,6,10-dodecatrien-1,5,8,12-tetrol, T-60363

$C_{15}H_{26}O_5$
9,12-Dioxododecanoic acid; Me ester, ethylene acetal, *in* D-60471
Lapidolinol, L-60015
1,4,6,9-Tetrahydroxydihydro-β-agarofuran, T-80090

$C_{15}H_{26}O_6$
1,4,6,9,15-Pentahydroxydihydro-β-agarofuran, P-80032

$C_{15}H_{26}O_7$
ent-5α,11-Epoxy-1β,4α,6α,8α,9β,14-eudesmanehexol, E-60018

$C_{15}H_{26}O_8$
1,2,4,6,8,9,14-Heptahydroxydihydro-β-agarofuran, H-80027

$C_{15}H_{27}N$
7-Amino-2,10-bisaboladiene, A-70096
7-Amino-3,10-bisaboladiene, A-60096
Tri-*tert*-butylazete, T-60249

$C_{15}H_{27}NO$
7-Amino-2,11-biaboladien-10*R*-ol, *in* A-70096
7-Amino-2,9-bisaboladien-11-ol, *in* A-70096
7-Amino-2,11-bisaboladien-10*S*-ol, *in* A-70096

$C_{15}H_{27}N_3$
3,5,12-Triazatetracyclo[5.3.1.1^{2,6}.0^{4,9}]dodecane; 3,5,12-Tri-Et, *in* T-70206
Tri-*tert*-butyl-1,2,3-triazine, T-60250

$C_{15}H_{28}O$
▷ Cyclopentadecanone, C-60219
10-Pentadecenal, P-80024

$C_{15}H_{28}O_2$
10-Bisabolene-7,15-diol, B-80135
2-Bisabolene-1,12-diol, B-70126
5-Decen-1-ol; 3-Methylbutanoyl, *in* D-70019
9-Dodecen-1-ol; Propanoyl, *in* D-70537

1,11-Eudesmanediol, E-70062
5,11-Eudesmanediol, E-70063
5,11-Eudesmanediol, E-80082

$C_{15}H_{28}O_3$
11-Bisabolene-7,10,15-triol, B-80136
12-Hydroxy-13-tetradecenoic acid; Me ester, *in* H-60229
2,6,10-Trimethyl-6,11-dodecadiene-2,3,10-triol, T-60362

$C_{15}H_{29}NO$
Cyclopentadecanone; Oxime, *in* C-60219

$C_{15}H_{30}$
3-*tert*-Butyl-2,2,4,5,5-tetramethyl-3-hexene, B-60350

$C_{15}H_{30}N_2O_3$
4,7,13-Trioxa-1,10-diazabicyclo[8.5.5]icosane, T-60375

$C_{15}H_{30}O_2$
Lardolure, *in* T-60372
2,4,6,8-Tetramethylundecanoic acid, T-60157

$C_{15}H_{30}O_4$
3,9-Dihydroxytetradecanoic acid; Me ester, *in* D-80386
12-Oxododecanoic acid; Me ester, Di-Me acetal, *in* O-60066

$C_{15}H_{30}O_6$
1,3,5-Tris(dimethoxymethyl)cyclohexane, *in* C-70226

$C_{15}H_{32}O$
3,7,11-Trimethyl-1-dodecanol, T-70282

$C_{15}H_{33}NO_6$
2-(2-Methoxyethoxy)-*N*,*N*-bis[2-(2-methoxyethoxy)ethyl]ethanamine, *in* T-70323

$C_{15}H_{33}N_3$
Hexahydro-1,3,5-triazine; 1,3,5-Tri-*tert*-butyl±, *in* H-60060

$C_{15}H_{35}N_5$
1,5,9,13,17-Pentaazacycloeicosane, P-60018

$C_{15}H_{36}O_3$
10,15-Dihydroxy-4-oplopanone, D-80348

$C_{16}H_4N_4S_2$
2,2′-(4,8-Dihydrobenzo[1,2-*b*:5,4-*b*′]dithiophene-4,8-diylidene)bispropanedinitrile, D-60196

$C_{16}H_8Br_2$
1,8-Dibromopyrene, D-70099
4,9-Dibromopyrene, D-80098

$C_{16}H_8Cl_2O_2$
1,8-Anthracenedicarboxylic acid; Dichloride, *in* A-60281

$C_{16}H_8Cl_4$
1,4,5,8-Tetrachloro-9,10-anthraquinodimethane, T-60026

$C_{16}H_8F_8$
4,5,7,8,12,13,15,16-Octafluoro[2.2]paracyclophane, O-60010

$C_{16}H_8N_2$
1,8-Dicyanoanthracene, *in* A-60281

$C_{16}H_8N_2O_4S$
2,2′-Thiobis-1*H*-isoindole-1,3(2*H*)-dione, T-70176

$C_{16}H_8N_2O_4S_2$
2,2′-Dithiobis-1*H*-isoindole-1,3(2*H*)-dione, D-70522
Dithiobisphthalimide, D-60508

$C_{16}H_8O_2$
Cyclohept[*fg*]acenaphthylene-5,6-dione, C-60194
Cyclohept[*fg*]acenaphthylene-5,8-dione, C-60195
Cycloocta[*def*]biphenylene-1,4-dione, C-80186

$C_{16}H_8O_3$
Benzo[*b*]naphtho[2,1-*d*]furan-5,6-dione, B-60033
Benzo[*b*]naphtho[2,3-*d*]furan-6,11-dione, B-60034
3,4-Phenanthrenedicarboxylic acid; Anhydride, *in* P-60068

$C_{16}H_8S_2$
Fluorantheno[3,4-*cd*]-1,2-dithiole, F-60017

$C_{16}H_8Se_2$
Fluorantheno[3,4-*cd*]-1,2-diselenole, F-60015

$C_{16}H_8Te_2$
Fluorantheno[3,4-*cd*]-1,2-ditellurole, F-60016

$C_{16}H_9ClO_2S$
1-Pyrenesulfonic acid; Chloride, *in* P-60210

$C_{16}H_9NO_2$
▷ 1-Nitropyrene, N-60040
2-Nitropyrene, N-60041
4-Nitropyrene, N-60042

$C_{16}H_9NO_2S$
3-(2-Benzothiazolyl)-2*H*-1-benzopyran, B-70056

$C_{16}H_9NO_3$
▷ 2-Nitro-1-pyrenol, N-80058

$C_{16}H_{10}$
Acephenanthrylene, A-70018
Benzo[*a*]biphenylene, B-60016
Benzo[*b*]biphenylene, B-60017
Dicyclopenta[*ef*,*kl*]heptalene, D-60167

$C_{16}H_{10}ClN$
1-Chlorobenzo[*a*]carbazole, C-80039

$C_{16}H_{10}F_3NO_2$
7-Amino-4-(trifluoromethyl)-2*H*-1-benzopyran-2-one; *N*-Ph, *in* A-60265

$C_{16}H_{10}F_6I_2O_5$
μ-Oxodiphenylbis(trifluoroacetato-*O*)diiodine, O-60065

$C_{16}H_{10}N_2$
Quino[7,8-*h*]quinoline, Q-70007

$C_{16}H_{10}N_2O_2$
Quino[7,8-*h*]quinoline-4,9(1*H*,12*H*)dione, Q-60007

$C_{16}H_{10}N_2S_2$
Thiazolo[4,5-*b*]quinoline-2(3*H*)-thione; 3-Ph, *in* T-60201

$C_{16}H_{10}N_6$
2,2′-Azodiquinoxaline, A-60353

$C_{16}H_{10}N_8$
21*H*,23*H*-Porphyrazine, P-70109

$C_{16}H_{10}O$
Anthra[1,2-*c*]furan, A-70217
Cyclobuta[*b*]anthracen-1(2*H*)one, C-80174
Phenanthro[9,10-*b*]furan, P-60073
Phenanthro[1,2-*c*]furan, P-70050
Phenanthro[3,4-*c*]furan, P-70051
Phenanthro[9,10-*c*]furan, P-60074

$C_{16}H_{10}O_2$
Benzo[*b*]naphtho[2,3-*e*][1,4]dioxan, B-80026
4,5:9,10-Diepoxy-4,5,9,10-tetrahydropyrene, D-70152
4*b*,9*a*-Dihydroindeno[1,2-*a*]indene-9,10-dione, D-70219
4*b*,9*b*-Dihydroindeno[2,1-*a*]indene-5,10-dione, D-70220
3-Phenyl-1,2-naphthoquinone, P-60120
4-Phenyl-1,2-naphthoquinone, P-60121

$C_{16}H_{10}O_3$
5-Formyl-4-phenanthrenecarboxylic acid, F-60074

$C_{16}H_{10}O_3S$
5-Hydroxy-2-(phenylthio)-1,4-naphthoquinone, H-70213
5-Hydroxy-3-(phenylthio)-1,4-naphthoquinone, H-70214
4-Oxo-2-phenyl-4*H*-1-benzothiopyran-3-carboxylic acid, O-60087
1-Pyrenesulfonic acid, P-60210
2-Pyrenesulfonic acid, P-60211
4-Pyrenesulfonic acid, P-60212

$C_{16}H_{10}O_3Se_2$
2,3-Bis(phenylseleno)-2-butenedioic acid; Anhydride, *in* B-80159

$C_{16}H_{10}O_4$
1,8-Anthracenedicarboxylic acid, A-60281
4-Oxo-2-phenyl-4*H*-1-benzopyran-3-carboxylic acid, O-60085
4-Oxo-3-phenyl-4*H*-1-benzopyran-2-carboxylic acid, O-60086
1,8-Phenanthrenedicarboxylic acid, P-80078
3,4-Phenanthrenedicarboxylic acid, P-60068

$C_{16}H_{10}O_5$
Corylinal, C-80153
Flaccidinin, F-80009
5-Hydroxy-6,7-methylenedioxyflavone, *in* T-60322
7-Hydroxy-3′,4′-methylenedioxyisoflavone, H-80203
Mutisifurocoumarin, M-70161

$C_{16}H_{10}O_6$
Bowdichione, B-70175
3,7-Dihydroxy-9-methoxycoumestan, *in* T-80294
3,8-Dihydroxy-9-methoxycoumestan, *in* T-80295
3,9-Dihydroxy-2-methoxycoumestone, *in* T-70249
9,10-Dihydroxy-5-methoxy-2*H*-pyrano[2,3,4-*kl*]xanthen-9-one, *in* T-70273
4′,5-Dihydroxy-6,7-methylenedioxyisoflavone, D-80341
2′,5-Dihydroxy-6,7-methylenedioxyisoflavone, *in* T-60107
2′,7-Dihydroxy-3′,4′-methylenedioxyisoflavone, *in* T-80105
5,7-Dihydroxy-3′,4′-methylenedioxyisoflavone, *in* T-80109
7-Hydroxy-3-(2-hydroxy-4,5-methylenedioxyphenyl)coumarin, *in* H-80261

$C_{16}H_{10}O_7$
5-Hydroxybowdichione, *in* B-70175
5,11,12-trihydroxy-7-methoxycoumestan, *in* T-80087
3,6,8-Trihydroxy-1-methylanthraquinone-2-carboxylic acid, T-60332
3,6,8-Trihydroxy-1-methylanthraquinone-2-carboxylic acid, T-80323
Variolaric acid, V-80004

$C_{16}H_{10}O_8$
Nasutin *C*, *in* E-70007

$C_{16}H_{11}ClO$
1-Phenanthreneacetic acid; Chloride, *in* P-70046

$C_{16}H_{11}F_3O_5S$
2,5-Diphenyl-1,3-dioxol-1-ium; Trifluoromethanesulfonate, *in* D-70478

$C_{16}H_{11}N$
1-(Cyanomethyl)phenanthrene, *in* P-70046
9-Cyanomethylphenanthrene, *in* P-70047
2*H*-Dibenz[*e*,*g*]isoindole, D-70067
Indolo[1,7-*ab*][1]benzazepine, I-60034
5*H*-Indolo[1,7-*ab*][1]benzazepine, I-80014

$C_{16}H_{11}NO$
1-Benzoylisoquinoline, B-60059
3-Benzoylisoquinoline, B-60060
4-Benzoylisoquinoline, B-60061

$C_{16}H_{11}NO_2$
2-Phenyl-4-(phenylmethylene)-5(4*H*)-oxazolone, P-60128

$C_{16}H_{11}NO_3$
1-Amino-8-hydroxyanthraquinone; *N*-Ac, *in* A-60177

$C_{16}H_{11}NO_4$
1-Amino-2-hydroxyanthraquinone; *N*-Ac, *in* A-60174
1-Amino-5-hydroxyanthraquinone; *N*-Ac, *in* A-60176

$C_{16}H_{11}N_3OS$
12*H*-Quinoxalino[2,3-*b*][1,4]benzothiazine; *N*-Ac, *in* Q-70008

$C_{16}H_{11}N_3O_2$
12*H*-Quinoxalino[2,3-*b*][1,4]benzoxazine; *N*-Ac, *in* Q-70009

$C_{16}H_{12}$
Cyclohepta[*ef*]heptalene, C-60197
Cycloocta[*a*]naphthalene, C-70234
Cycloocta[*b*]naphthalene, C-70235
2,6-Dihydroaceanthrylene, D-80169
1,10-Dihydrodicyclopenta[*a,h*]naphthalene, D-60220
3,8-Dihydrodicyclopenta[*a,h*]naphthalene, D-60221
9,10-Dihydro-9,10-dimethyleneanthracene, D-70194
5,10-Dihydroindeno[2,1-*a*]indene, D-70218
5-Methylene-5*H*-dibenzo[*a,d*]cycloheptene, M-80084
[2.2]Paracyclophadiene, P-70007
4*b*,8*b*,8*c*,8*d*-Tetrahydrodibenzo[*a,f*]cyclopropa[*cd*]pentalene, T-80057

$C_{16}H_{12}Cl_2N_4O$
4-(2,5-Dichlorophenylhydrazono)-5-methyl-2-phenyl-3*H*-pyrazol-3-one, D-70138

$C_{16}H_{12}Cl_2O_2$
Bibenzyl-2,2′-dicarboxylic acid; Dichloride, *in* B-80071

$C_{16}H_{12}Cl_2O_5$
2,4-Dichloro-1-hydroxy-5,8-dimethoxyxanthone, *in* T-70181

$C_{16}H_{12}F_2O_4$
4,4′-Difluoro-[1,1′-biphenyl]-3,3′-dicarboxylic acid; Di-Me ester, *in* D-60178
4,5-Difluoro-[1,1′-biphenyl]-2,3-dicarboxylic acid; Di-Me ester, *in* D-60179
6,6′-Difluoro-[1,1′-biphenyl]-2,2′-dicarboxylic acid; Di-Me ester, *in* D-60180

$C_{16}H_{12}F_4$
4,5,7,8-Tetrafluoro[2.2]paracyclophane, T-60050

$C_{16}H_{12}N_2$
2,2′-Bis(cyanomethyl)biphenyl, *in* B-60115
4,4′-Bis(cyanomethyl)biphenyl, *in* B-60116
2,4-Diphenylpyrimidine, D-70494
4,5-Diphenylpyrimidine, D-70495
4,6-Diphenylpyrimidine, D-70496

$C_{16}H_{12}N_2O$
1-Benzoylisoquinoline; Oxime, *in* B-60059
4,5-Diphenylpyrimidine; 1-Oxide, *in* D-70495
4,6-Diphenylpyrimidine; *N*-Oxide, *in* D-70496

$C_{16}H_{12}N_2O_2$
2,2′-Dicyanobibenzyl, *in* B-80071
4*b*,9*b*-Dihydroindeno[2,1-*a*]indene-5,10-dione; Dioxime, *in* D-70220

$C_{16}H_{12}N_2O_7S_2$
6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid, H-80255

$C_{16}H_{12}N_4$
Dibenzo[*b,g*][1,8]naphthyridine-11,12-diamine, D-80071

$C_{16}H_{12}O$
1-Acetylanthracene, A-70030
2-Acetylanthracene, A-70031
9-Anthraceneacetaldehyde, A-60280
Octaleno[3,4-*c*]furan, O-70019
1-Phenyl-2-naphthol, P-60115
3-Phenyl-2-naphthol, P-60116
4-Phenyl-2-naphthol, P-60117
5-Phenyl-2-naphthol, P-60118
8-Phenyl-2-naphthol, P-60119

$C_{16}H_{12}O_2$
5-(2,4,6-Cycloheptatrien-1-ylideneethylidene)-3,6-cycloheptadiene-1,2-dione, C-70222
2,3-Dihydro-3-(phenylmethylene)-4*H*-1-benzopyran-4-one, D-60263
1-Phenanthreneacetic acid, P-70046
9-Phenanthreneacetic acid, P-70047
Tricyclo[8.4.1.1^{3,8}]hexadeca-3,5,7,10,12,14-hexaene-2,9-dione, T-60264

$C_{16}H_{12}O_2S$
3-Methylthio-2-phenyl-4*H*-1-benzopyran-4-one, *in* M-60025

$C_{16}H_{12}O_3$
7-Hydroxy-2-methylisoflavone, H-80205
7-Hydroxy-3-methylisoflavone, H-80206
6-Methoxyflavone, *in* H-70130
7-Methoxyflavone, *in* H-70131
8-Methoxyflavone, *in* H-70132
5-Methoxy-4-phenanthrenecarboxylic acid, *in* H-80232
Nordracorhodin, N-70074

$C_{16}H_{12}O_4$
1,5-Biphenylenedicarboxylic acid; Di-Me ester, *in* B-80111
1,8-Biphenylenedicarboxylic acid; Di-Me ester, *in* B-80112
2,3-Biphenylenedicarboxylic acid; Di-Me ester, *in* B-80113
2,6-Biphenylenedicarboxylic acid; Di-Me ester, *in* B-80114
2,7-Biphenylenedicarboxylic acid; Di-Me ester, *in* B-80115
1,8-Biphenylenediol; Di-Ac, *in* B-80118
2,6-Biphenylenediol; Di-Ac, *in* B-80120
2,7-Biphenylenediol; Di-Ac, *in* B-80121
7-Hydroxy-3-(4-hydroxybenzylidene)-4-chromanone, H-60152
▷ 7-Hydroxy-4′-methoxyisoflavone, H-80190
Isodalbergin, I-60097
Vesparione, V-70007

$C_{16}H_{12}O_4Se_2$
2,3-Bis(phenylseleno)-2-butenedioic acid, B-80159

$C_{16}H_{12}O_5$
3-(3,4-Dihydroxybenzylidene)-7-hydroxy-4-chromanone, *in* D-70288
▷ 5,7-Dihydroxy-4′-methoxyflavone, D-70319
4′,7-Dihydroxy-3′-methoxyflavone, *in* T-80301
4′,5-Dihydroxy-7-methoxyisoflavone, D-80335
4′,7-Dihydroxy-5-methoxyisoflavone, D-80336
5,7-Dihydroxy-4′-methoxyisoflavone, D-80337
2′,7-Dihydroxy-4′-methoxyisoflavone, *in* T-80306
3′,7-Dihydroxy-4′-methoxyisoflavone, *in* T-80308
4′,6-Dihydroxy-7-methoxyisoflavone, *in* T-80310
4′,7-Dihydroxy-2′-methoxyisoflavone, *in* T-80306
4′,7-Dihydroxy-3′-methoxyisoflavone, *in* T-80308
4′,7-Dihydroxy-6-methoxyisoflavone, *in* T-80310
7,8-Dihydroxy-4′-methoxyisoflavone, *in* T-70265
7,8-Dihydroxy-4′-methoxyisoflavone, *in* T-80311
1,8-Dihydroxy-6-methoxy-2-methylanthraquinone, *in* T-70269
7-Hydroxy-3-(2-hydroxy-4-methoxyphenyl)coumarin, *in* D-80364
3-Hydroxy-2-hydroxymethyl-1-methoxyanthraquinone, *in* D-70306
2-(2-Hydroxy-4-methoxyphenyl)-5,6-methylenedioxybenzofuran, *in* D-80355
Maackiain, M-70001
Obtusifolin/, *in* T-80322
Oxoflaccidin, *in* F-80009
Pabulenone, *in* P-60170
2′,5,7-Trihydroxyflavone, T-80299
4′,5,7-Trihydroxy-6-methylflavone, T-80326

$C_{16}H_{12}O_6$
6*a*,12*a*-Dihydro-2,3,10-trihydroxy[2]benzopyrano[4,3-*b*][1]benzopyran-7(5*H*)-one, 9CI, *in* C-70200
3-(2,4-Dihydroxybenzoyl)-7,8-dihydroxy-1*H*-2-*benzopyran*, *in* P-70017
2-(2,4-Dihydroxy-3-methoxyphenyl)-5,6-methylenedioxybenzofuran, *in* D-80389
3,5-Dihydroxy-6,7-methylenedioxyflavanone, *in* T-60105
2′,7-Dihydroxy-4′,5′-methylenedioxyisoflavanone, *in* T-80101
3,4-Dihydroxy-8,9-methylenedioxypterocarpan, *in* T-80119
4-(3,4-Dihydroxyphenyl)-7-hydroxy-5-methoxycoumarin, *in* D-80356
Peltochalcone, P-70017
Rengasin, *in* A-80188
3,5,6,7-Tetrahydroxy-8-methylflavone, T-70117
3,5,7,8-Tetrahydroxy-6-methylflavone, T-70118
2′,5,7-Trihydroxy-6′-methoxyflavone, *in* T-50153
▷ 4′,5,7-Trihydroxy-6-methoxyisoflavone, T-80319
2′,3′,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80105
2′,4′,5-Trihydroxy-7-methoxyisoflavone, *in* T-80106
2′,4′,7-Trihydroxy-5-methoxyisoflavone, *in* T-80106
2′,5,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80106
3′,4′,5-Trihydroxy-7-methoxyisoflavone, *in* T-80109
3′,5,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80109
3′,5′,7-Trihydroxy-4′-methoxyisoflavone, *in* T-80110
3′,7,8-Trihydroxy-4′-methoxyisoflavone, *in* T-70112
4′,5,7-Trihydroxy-3′-methoxyisoflavone, *in* T-80109
4′,5,7-Trihydroxy-8-methoxyisoflavone, *in* T-80113
4′,7,8-Trihydroxy-6-methoxyisoflavone, *in* T-70113
1,3,5-Trihydroxy-4-methoxy-2-methylanthraquinone, *in* T-60112
1,3,8-Trihydroxy-5-methoxy-2-methylanthraquinone, *in* T-60113

$C_{16}H_{12}O_7$
Crombeone, C-70200
2′,3,5,8-Tetrahydroxy-7-methoxyflavone, *in* P-70029
3′,4′,5,7-Tetrahydroxy-8-methoxyisoflavone, *in* P-80045
3,6*a*,7-Trihydroxy-8,9-methylenedioxypterocarpan, *in* P-80056

$C_{16}H_{13}ClO_5$
2-Chloro-1-hydroxy-5,8-dimethoxy-6-methylxanthone, *in* T-70181
5-Chloro-8-hydroxy-1,4-dimethoxy-3-methylxanthone, *in* T-70181

$C_{16}H_{13}N$
5,10-Dihydroindeno[1,2-*b*]indole; N-Me, *in* D-80216

$C_{16}H_{13}NO$
2-Methoxy-4-phenylquinoline, *in* P-60131
4-Methoxy-2-phenylquinoline, *in* P-60132
1-Methyl-2-phenyl-4(1*H*)-*quinolinone*, *in* P-60132
9-Phenanthreneacetic acid; Amide, *in* P-70047

$C_{16}H_{13}NOS$
5-Methyl-2-phenyl-1,5-benzothiazepin-4(5*H*)-one, *in* P-60081

$C_{16}H_{13}NO_2$
10-Amino-9-anthracenecarboxylic acid; Me ester, *in* A-70088
Dibenz[*b,g*]azocine-5,7(6*H*,12*H*)-dione; *N*-Me, *in* D-60068
1*H*-Indole-3-carboxylic acid; *N*-Benzyl, *in* I-80012

$C_{16}H_{13}NO_5$
1-Amino-4,5-dihydroxy-7-methoxy-2-methylanthraquinone, A-60145

$C_{16}H_{13}NS$
10*H*-[1]Benzothieno[3,2-*b*]indole; *N*-Et, *in* B-70059

$C_{16}H_{14}$
9-Benzylidene-1,3,5,7-cyclononatetraene, B-60069
1,6:7,12-Bismethano[14]annulene, B-60165
9,10-Dihydro-9,10-ethanoanthracene, D-70207
10,11-Dihydro-5-methylene-5*H*-dibenzo[*a*,*d*]cycloheptene, D-80219
4,5-Dimethylphenanthrene, D-60439
1,1-Diphenyl-1,3-butadiene, D-70476
11*b*-Methyl-11*bH*-Cyclooct[*cd*]azulene, M-60060
7,8,9,10-Tetrahydrofluoranthene, T-70061
4,5,9,10-Tetrahydropyrene, T-60083

$C_{16}H_{14}N_2$
1,2-Dihydro-4,6-diphenylpyrimidine, D-60235

$C_{16}H_{14}N_2O$
1-(1-Isoquinolinyl)-1-(2-pyridinyl)ethanol, I-60134

$C_{16}H_{14}N_2O_2$
2,3-Diaminobiphenylene; N,N′-Di-Ac, *in* D-80054
2,6-Diaminobiphenylene; N,N′-Di-Ac, *in* D-80055
5,6-Dihydrobenzo[*c*]cinnoline; Di-Ac, *in* D-80172
2-Phenyl-3*H*-indol-3-one; *N*-Oxide, oxime, Et ether, *in* P-60114

$C_{16}H_{14}N_2O_3$
2,3-Dihydro-2-hydroxy-1*H*-imidazole-4,5-dione; 1,3-Di-Ph, Me ether, *in* D-60243

$C_{16}H_{14}N_2S_2$
2,5-Dihydro-4,6-pyrimidinedithiol; Di-Ph thioether, *in* D-70257

$C_{16}H_{14}N_4$
3,3′-Dimethyl-2,2′-biindazole, D-80421
5,5′-Dimethyl-2,2′-biindazole, D-80422
7,7′-Dimethyl-2,2′-biindazole, D-80423

$C_{16}H_{14}O$
2-(9-Anthracenyl)ethanol, A-60282
3,4-Dihydro-2-phenyl-1(2*H*)-naphthalenone, D-60265
3,4-Dihydro-3-phenyl-1(2*H*)-naphthalenone, D-60266
3,4-Dihydro-4-phenyl-1(2*H*)-naphthalenone, D-60267
10,10-Dimethyl-9(10*H*)-anthracenone, D-60403
2,3-Diphenyl-2-butenal, D-60475
2,4-Diphenyl-3-butyn-1-ol, D-80508
3,3-Diphenylcyclobutanone, D-60476

$C_{16}H_{14}OS$
▷ 2,3-Dihydro-5,6-diphenyl-1,4-oxathiin, D-70203

$C_{16}H_{14}OS_2$
1-(Phenylsulfinyl)-2-(phenylthio)cyclobutene, *in* B-70156

$C_{16}H_{14}O_2$
Dihydro-2,2-diphenyl-2(3*H*)-furanone, D-80197
Dihydro-3,3-diphenyl-2(3*H*)-furanone, D-80198
Dihydro-3,4-diphenyl-2(3*H*)-furanone, D-80199
Dihydro-3,5-diphenyl-2(3*H*)-furanone, D-80200
Dihydro-4,4-diphenyl-2(3*H*)-furanone, D-80201
Dihydro-4,5-diphenyl-2(3*H*)-furanone, D-80202
Dihydro-5,5-diphenyl-2(3*H*)-furanone, D-80203
4,5-Dimethoxyphenanthrene, *in* P-70048
2,2-Diphenyl-4-methylene-1,3-dioxolane, D-70486
Dracaenone, D-70546
3,6-Phenanthrenedimethanol, P-60069
4,5-Phenanthrenedimethanol, P-60070

$C_{16}H_{14}O_2S_2$
1,2-Bis(phenylsulfinyl)cyclobutene, *in* B-70156

$C_{16}H_{14}O_3$
2-Benzoylbenzoic acid; Et ester, *in* B-80054
3,7-Dimethoxy-2-phenanthrenol, *in* T-60339

$C_{16}H_{14}O_3S_2$
1-(Phenylsulfinyl)-2-(phenylsulfonyl)cyclobutene, *in* B-70156

$C_{16}H_{14}O_4$
Amoenumin, A-80150
Bibenzyl-2,2′-dicarboxylic acid, B-80071
[1,1′-Biphenyl]-2,2′-diacetic acid, B-60115
[1,1′-Biphenyl]-4,4′-diacetic acid, B-60116
2′,4-Dihydroxy-4′-methoxychalcone, *in* D-80367
4′,7-Dihydroxy-2′-methoxyisoflavene, *in* T-80305
1-(2,4-Dihydroxy-6-methoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
1,5-Dimethoxy-2,7-phenanthrenediol, *in* T-80114
3,4-Dimethoxy-2,7-phenanthrenediol, *in* T-80115
5,7-Dimethoxy-2,3-phenanthrenediol, *in* T-60120
5,7-Dimethoxy-2,6-phenanthrenediol, *in* T-80115
5,5′-(1,2-Ethanediyl)bis-1,3-benzodioxole, *in* T-60101
Ferulidene, *in* X-60002
Flaccidin, F-70010
Flaccidin, *in* F-80009
7-Hydroxy-4′-methoxyisoflavanone, *in* D-80322
2-(4-Hydroxy-2-methoxyphenyl)-6-methoxybenzofuran, *in* D-80363
9-Hydroxy-3-methoxypterocarpan, *in* D-60373

$C_{16}H_{14}O_4S$
2,2′-Thiobisbenzoic acid; Di-Me ester, *in* T-70174
4,4′-Thiobisbenzoic acid; Di-Me ester, *in* T-70175

$C_{16}H_{14}O_4S_2$
1,2-Bis(phenylsulfonyl)cyclobutene, *in* B-70156
5-(3,4-Diacetoxy-1-butynyl)-2,2′-bithienyl, *in* B-80166

$C_{16}H_{14}O_5$
Demethylfrutescin 1′-ylacetate, *in* H-80231
Dibenzyl dicarbonate, *in* D-70111
3-(3,4-Dihydroxybenzyl)-7-hydroxy-4-chromanone, D-70288
5,8-Dihydroxy-7-methoxyflavanone, *in* T-60321
2′,7-Dihydroxy-4′-methoxyisoflavanone, *in* T-80303
3′,7-Dihydroxy-4′-methoxyisoflavanone, *in* T-70263
5,7-Dihydroxy-4′-methoxyisoflavanone, *in* T-80304
3,6*a*-Dihydroxy-9-methoxypterocarpan, *in* T-80337
6*a*,9-Dihydroxy-3-methoxypterocarpan, *in* T-80337
3,10-Dihydroxy-9-methoxypterocarpan, *in* T-80338
3,4-Dihydroxy-9-methoxypterocarpan, *in* T-80336
3,9-Dihydroxy-10-methoxypterocarpan, *in* T-80338
2′,7-Dihydroxy-4′,5′-methylenedioxyisoflavan, *in* T-80097
2-(2,4-Dihydroxyphenyl)-5,6-dimethoxybenzofuran, *in* D-80355
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)-2-propen-1-one, *in* D-80362
2-(3-Hydroxy-2,4-dimethoxyphenyl)-6-benzofuranol, *in* H-80260
6-Hydroxy-2-(4-hydroxy-2,3-dimethoxyphenyl)benzofuran, *in* H-80260
Isogosferol, *in* X-60002
3-(4-Methoxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, *in* H-80245
Moracin *F*, *in* M-60146
Pabularinone, *in* P-60170
Pabulenol, P-60170
Sainfuran, S-60002
2′,3′,7-Trihydroxy-4′-methoxyisoflavene, *in* T-80103
2′,4,7-Trihydroxy-3′-methoxyisoflavene, *in* T-80103
1,3,7-Trimethoxyxanthone, *in* T-80347

$C_{16}H_{14}O_6$
Anhydrofusarubin 9-methyl ether, *in* F-60108
3-(3,4-Dihydroxybenzyl)-3,7-dihydroxy-4-chromanone, *in* D-70288
5,8-Dihydroxy-2,3-dimethyl-1,4-naphthoquinone; Di-Ac, *in* D-60317
2,3-Dihydroxy-2,3-diphenylbutanedioic acid, D-80312
1-(2,4-Dihydroxy-3-methoxyphenyl)-3-(3,4-dihydroxyphenyl)-2-propen-1-one, *in* D-80372
Diphenyl tartrate, *in* T-70005
6,6′-(1,2-Ethanediyl)bis-1,3-benzodioxol-4-ol, *in* H-60062
3-Hydroxy-1,2,4-trimethoxyxanthone, *in* T-60126
7-Hydroxy-2,3,4-trimethoxyxanthone, *in* T-60128
8-Hydroxy-1,3,5-trimethoxyxanthone, *in* T-70123
1,4,5-Naphthalenetriol; Tri-Ac, *in* N-60005
2′,5,8-Trihydroxy-7-methoxyflavanone, *in* T-70104
4′,5,7-Trihydroxy-2′-methoxyisoflavanone, *in* T-80100
3,6a,7-Trihydroxy-9-methoxypterocarpan, *in* T-80120

$C_{16}H_{14}O_6S$
4,4′-Thiobisbenzoic acid; Di-Me ester, *S*-dioxide, *in* T-70175

$C_{16}H_{14}O_7$
5,10-Dihydroxy-1,7-dimethoxy-3-methyl-1*H*-naphtho[2,3-*c*]pyran-6,9-dione, *in* T-80320
3′,5-Dihydroxy-4′,6,7-trimethoxyflavanone, *in* P-70028
1,8-Dihydroxy-2,3,6-trimethoxyxanthone, *in* P-70036
3,6-Dihydroxy-1,2,3-trimethoxyxanthone, *in* P-70036
3,8-Dihydroxy-1,2,4-trimethoxyxanthone, *in* P-60051
6,8-Dihydroxy-1,2,5-trimethoxyxanthone, *in* P-60052
Isolecanoric acid, I-60103
Nectriafurone; 8-Me ether, *in* N-60016
3′,4′,5,7-Tetrahydroxy-6-methoxyflavanone, *in* P-70028
Ventilone *E*, *in* V-60004

$C_{16}H_{14}S_2$
1,2-Bis(phenylthio)cyclobutene, B-70156

$C_{16}H_{14}Se$
2,5-Dihydro-3,4-diphenylselenophene, D-70205
Distyryl selenide, D-60503

$C_{16}H_{15}Br$
1-Bromomethyl-2,3-diphenylcyclopropane, B-80214

$C_{16}H_{15}ClO_4S$
4-Phenyl-2*H*-1-benzothiopyran; S-Me, perchlorate, *in* P-80092

$C_{16}H_{15}ClO_6$
Lonapalene, *in* C-60118

$C_{16}H_{15}N$
7,12-Dihydro-5*H*-6,12-methanodibenz[*c*,*f*]azocine, D-60255
2,3-Diphenylbutanoic acid; Nitrile, *in* D-80506

$C_{16}H_{15}NO$
9-Amino-9,10-dihydroanthracene; *N*-Ac, *in* A-60136

2-Amino-9,10-dihydrophenanthrene; *N*-Ac, *in* A-60141
9-Amino-9,10-dihydrophenanthrene; *N*-Ac, *in* A-60143
10,11-Dihydro-5*H*-dibenz[*b,f*]azepine; 5-Ac, *in* D-70185
3,4-Dihydro-4-phenyl-1(2*H*)-naphthalenone; Oxime, *in* D-60267
3,6-Dimethylcarbazole; *N*-Ac, *in* D-70387

$C_{16}H_{15}NOS$
2-Phenyl-1,5-benzothiazepin-4(5*H*)-one; 2,3-Dihydro, *N*-Me, *in* P-60081

$C_{16}H_{15}NO_2$
2-Amino-1,3-diphenyl-1-propanone; *N*-Formyl, *in* A-60149

$C_{16}H_{15}NO_2S$
10*H*-Phenothiazine-1-carboxylic acid; *N*-Et, Me ester, *in* P-70055
10*H*-Phenothiazine-3-carboxylic acid; *N*-Et, Me ester, *in* P-70057
10*H*-Phenothiazine-4-carboxylic acid; *N*-Et, Me ester, *in* P-70058

$C_{16}H_{15}NO_4$
4-Hydroxy-3,6-dimethoxy-2-methyl-9*H*-carbazole-1-carboxaldehyde, *in* H-70154
2,2′-Iminodibenzoic acid; Di-Me ester, *in* I-60014
2,4′-Iminodibenzoic acid; Di-Me ester, *in* I-60016
4,4′-Iminodibenzoic acid; Di-Me ester, *in* I-60018

$C_{16}H_{15}NO_5$
1-Amino-2,7-naphthalenediol; O,O,N-Tri Ac, *in* A-80113
4-Amino-1,3-naphthalenediol; O,O,N-Tri-Ac, *in* A-80118
2-Amino-1,4-naphthalenediol; *O,O,N*-Tri-Ac, *in* A-80114
2-Amino-1,6-naphthalenediol; *O,O,N*-Tri-Ac, *in* A-80115
4-Amino-1,2-naphthalenediol; *O,O,N*-Tri-Ac, *in* A-80117

$C_{16}H_{15}N_3O_2$
1,8-Diaminocarbazole; 1,8-*N*-Di-Ac, *in* D-80056

$C_{16}H_{15}N_5$
2,4-Diamino-6-methyl-1,3,5-triazine; *N,N*-Di-Ph, *in* D-60040
2,4-Diamino-6-methyl-1,3,5-triazine; *N,N′*-Di-Ph, *in* D-60040

$C_{16}H_{16}$
9,10-Dihydro-9,9-dimethylanthracene, D-60224
4,5-Dimethylphenanthrene; 9,10-Dihydro, *in* D-60439
Heptacyclo[7.7.0.0^{2,6}.0^{3,15}.0^{4,12}.0^{5,10}.0^{11,16}]hexadeca-7,13-diene, H-70011
1,6,8-Hexadecatriene-10,12,14-triyne, H-80043
1,2,3,6,7,8-Hexahydropyrene, H-70069
1,2,3,3*a*,4,5-Hexahydropyrene, H-70068

$C_{16}H_{16}N_2$
10,10-Dimethyl-9(10*H*)-anthracenone; Hydrazone, *in* D-60403

$C_{16}H_{16}N_2O_2$
2,2′-Diaminobiphenyl; 2,2′-*N*-Di-Ac, *in* D-60033
5,5′-Diamino-2,2′-biphenyldicarboxylic acid; Di-Me ester, *in* D-80051
Methylpropanedioic acid; Dianilide, *in* M-80149

$C_{16}H_{16}N_2O_3$
2,4,6-Trimethyl-3-nitroaniline; *N*-Benzoyl, *in* T-70285

$C_{16}H_{16}N_2O_4$
[2,2′-Bipyridine]-6,6′-dicarboxylic acid; Di-Et ester, *in* B-60128
2,2′-Diamino-4,4′-biphenyldicarboxylic acid; Di-Me ester, *in* D-80046

$C_{16}H_{16}N_4O_5S$
6-Nitro-1-[[(2,3,5,6-tetramethylphenyl)sulfonyl]oxy]-1*H*-benzotriazole, N-80060

$C_{16}H_{16}O$
1,3-Diphenyl-2-butanone, D-80507
6,7,8,9-Tetrahydro-6-phenyl-5*H*-benzocyclohepten-5-one, T-60080

$C_{16}H_{16}O_2$
2,2′-Dihydroxystilbene; Di-Me ether, *in* D-80378
3,5-Dihydroxystilbene; Di-Me ether, *in* D-80384
4,4′-Dihydroxystilbene; Di-Me ether, *in* D-80385
2,3-Diphenylbutanoic acid, D-80506
2,2-Diphenylpropanoic acid; Me ester, *in* D-70493
2,3-Naphthalenedicarboxylic acid; Di-Et ester, *in* N-80001
3,3′,5,5′-Tetramethyl[bi-2,5-cyclohexadien-1-ylidene]-4,4′-dione, T-80140

$C_{16}H_{16}O_3$
3-(1,1-Dimethyl-2-propenyl)-4-hydroxy-6-phenyl-2*H*-pyran-2-one, D-70434
Echinofuran *B*, *in* E-60002
5-[2-(3-Methoxyphenyl)ethyl]-1,3-benzodioxole, *in* T-60316
9-Methylcyclolongipesin, *in* C-60214

$C_{16}H_{16}O_4$
8-Acetoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene, *in* H-70042
Angolensin, A-80155
5,7-Azulenedicarboxylic acid; Di-Et ester, *in* A-70295
9,10-Dihydro-5,6-dihydroxy-2,4-dimethoxyphenanthrene, *in* D-70247
9,10-Dihydro-2,5-dimethoxy-1,7-phenanthrenediol, *in* T-80114
9,10-Dihydro-2,7-dimethoxy-1,5-phenanthrenediol, *in* T-80114
9,10-Dihydro-3,4-dimethoxy-2,7-phenanthrenediol, *in* T-80115
2′,4′-Dihydroxy-7-methoxyisoflavan, *in* T-80302
4′,7-Dihydroxy-2′-methoxyisoflavan, *in* T-80302
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-1-propanone, *in* T-80332
Gleinadiene, *in* G-60023
Homocyclolongipesin, H-60088
3-(4-Hydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* D-80366
Perforatin *A*, *in* A-60075
6,7,14,15-Tetrahydrodibenzo[*b,h*][1,4,7,10]tetraoxacyclododecin, T-80059
2,4,6-Trimethoxybenzophenone, *in* T-80285

$C_{16}H_{16}O_5$
Citreofuran, C-80136
trans-Dehydrocurvularin, *in* C-80166
Deoxyaustrocortilutein, *in* A-60321
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone, *in* H-80244
3-(2,4-Dihydroxy-6-methoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* H-80243
6-[2-(3,4-Dimethoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one, *in* H-70122
3-(4-Hydroxyphenyl)-1-(2,4-dihydroxy-6-methoxyphenyl)-1-propanone, *in* H-80246
Pranferol, *in* P-60170
Shikonin, S-70038

$C_{16}H_{16}O_6$
Altersolanol *B*, *in* A-60080
Austrocortilutein, A-60321
Deoxyaustrocortirubin, *in* A-60322
3-(3,4-Dihydroxybenzyl-3,4,7-trihydroxychroman, *in* D-70288
Epicatechin; *O*$^{3'}$-Me, *in* P-70026
Fonsecin B, *in* F-80073
Meciadanol, *in* P-70026
1,4,5,7-Naphthalenetetrol; 4,5-Di-Me ether, di-Ac, *in* N-80003
3,3′,5,7-Tetrahydroxy-4′-methoxyflavan, *in* P-70026

$C_{16}H_{16}O_7$
Altersolanol *C*, *in* A-60080
Austrocortirubin, A-60322
Fusarubin; *O*^{9}-Me, *in* F-60108
Fusarubin methyl acetal, *in* F-60108
1,2,3,4-Tetrahydro-1,2,4,5-tetrahydroxy-7-methoxy-2-methylanthraquinone, T-80078

$C_{16}H_{16}O_8$
Altersolanol *A*, A-60080
4-*O*-Caffeoylshikimic acid, C-80006
5-*O*-Caffeoylshikimic acid, C-80007

$C_{16}H_{16}S_2$
2,11-Dithia[3.3]paracyclophane, D-60505
5,7,12,14-Tetrahydrodibenzo[*c,h*][1,6]dithiecin, T-80058

$C_{16}H_{17}N$
Azetidine; *N*-Benzhydryl, *in* A-70283
1,2,3,4-Tetrahydroquinoline; *N*-Benzyl, *in* T-70093

$C_{16}H_{17}NO$
2,3-Diphenylbutanoic acid; Amide, *in* D-80506
1,3-Diphenyl-2-butanone; Oxime, *in* D-80507

$C_{16}H_{17}NO_3$
4-Hydroxy-3,6-dimethoxy-1,2-dimethylcarbazole, *in* T-70253

$C_{16}H_{17}O_4$
9,10-Dihydro-2,7-dihydroxy-3,5-dimethoxyphenanthrene, *in* T-60120

$C_{16}H_{18}N_2$
[3](2.2)[3](5.5)Pyridinophane, P-60227
[3](2.5)[3](5.2)Pyridinophane, P-60228
[3.3][2.6]Pyridinophane, P-60226

$C_{16}H_{18}N_2O$
N-Ethyl-*N′*-methyl-*N,N′*-diphenylurea, *in* D-70499
5-Phenyl-3-pyridinecarboxylic acid; Diethylamide, *in* P-80129

$C_{16}H_{18}O$
6,8,14-Hexadecatriene-10,12-diyn-1-al, H-80042

$C_{16}H_{18}O_2$
13-Acetoxy-9-tetradecene-2,4,6-triyne, *in* T-80042
2,3-Diphenyl-2,3-butanediol, D-80505
Methyl 8-isopropyl-5-methyl-2-naphthalenecarboxylate, *in* I-60129
4,6,12-Tetradecatrien-8,10-diyn-1-ol; Ac, *in* T-80032

$C_{16}H_{18}O_3$
Heritonin, H-80034
3-Hydroxy-3′,4-dimethoxybibenzyl, *in* T-60316
8-Methoxy-1(6),2,4,7(11)-cadinatetraen-12,8-olide, *in* H-70114
4-Methoxy-3-(3-methyl-2-butenyl)-5-phenyl-2(5*H*)-furanone, M-70047

$C_{16}H_{18}O_4$
8-Angeloyloxylachnophyllum ester, *in* H-80150
1-(3,4-Dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)ethane, *in* D-80359
3-(1,1-Dimethyl-2-propenyl)-7,8-dimethoxy-2*H*-1-benzopyran-2-one, D-80470
Gleinene, G-60023
1-(3-Hydroxy-5-methoxyphenyl)-2-(4-hydroxy-3-methoxyphenyl)ethane, *in* D-80361
4-[2-(3-Hydroxyphenyl)ethyl]-2,6-dimethoxyphenol, *in* T-60102
9-Methyllongipesin, M-70091
O-!Methylcedrelopsin, *in* C-60026
Rutacultin, R-80016
2,2′,3,4-Tetramethoxybiphenyl, *in* B-70122
2,2′,3,4-Tetramethoxybiphenyl, *in* B-80125
2,3,3′,4-Tetramethoxybiphenyl, *in* B-80126
2,3,4,4′-Tetramethoxybiphenyl, *in* B-70123
2,3,4,4′-Tetramethoxybiphenyl, *in* B-80127
2′,3,4,5-Tetramethoxybiphenyl, *in* B-80128

$C_{16}H_{18}O_5$
Arnebin V, *in* D-80343

cis-Dehydrocurvularin, *in* C-80166
Murracarpin, M-80197
Resorcylide, R-70001
Skimminin, S-60035

$C_{16}H_{18}O_6$
2-(1,4-Dihydroxy-4-methylpentyl)-5,8-dihydroxy-1,4-naphthoquinone, D-80343
Murraculatin, M-70158
12-Oxocurvularin, *in* C-80166
2,5,7-Trihydroxy-3-(5-hydroxyhexyl)-1,4-naphthoquinone, T-70262

$C_{16}H_{18}O_8$
3,6-Dimethyl-1,2,4,5-benzenetetracarboxylic acid; Tetra-Me ester, *in* D-60407

$C_{16}H_{18}O_9$
▷ 3-*O*-Caffeoylquinic acid, C-70005
Fabiatrin, *in* H-80189
Magnolioside, *in* H-80188
Scopolin, *in* H-80189

$C_{16}H_{19}N_3O_6$
Albomitomycin *A*, A-70080
Isomitomycin *A*, I-70070

$C_{16}H_{20}$
Heptacyclo[7.7.0.0^{2,6}.0^{3,15}.0^{4,12}.0^{5,10}.0^{11,16}]hexadecane, *in* H-70011

$C_{16}H_{20}Br_2O_2$
Cymobarbatol, C-80202
4-Isocymobarbatol, *in* C-80202

$C_{16}H_{20}ClN_3$
Bindschedler's green; Chloride, *in* B-60110

$C_{16}H_{20}N_2$
2,2′-Bis(dimethylamino)biphenyl, *in* D-60033
1,2-Diphenyl-1,2-ethanediamine; *N,N′*-Di-Me, *in* D-70480

$C_{16}H_{20}N_2O_6S_2$
N,N′-Bis(3-sulfonatopropyl)-2,2′-bipyridinium, B-70159
N,N′-Bis(3-sulfonatopropyl)-4,4′-bipyridinium, B-70160

$C_{16}H_{20}N_3^{\oplus}$
Bindschedler's green, B-60110

$C_{16}H_{20}O$
2-Phenyl-2-adamantanol, P-70060

$C_{16}H_{20}O_2$
14-Acetoxy-2,4,8,10-tetradecaen-6-yne, *in* T-80031
Methyl 3,4-dihydro-8-isopropyl-5-methyl-2-naphalenecarboxylate, *in* I-60129

$C_{16}H_{20}O_3$
14-Acetoxy-8,10-tetradecadiene-4,6-diyn-3-ol, *in* T-80026
Alliodorin, A-70083
6-Methoxy-1,3-primnatrienedione, *in* P-80174
Methyl 3-oxo-1,4(15),11(13)-eudesmatrien-12-oate, *in* H-80164

$C_{16}H_{20}O_4$
1-(5,7-Dihydroxy-2,2,6-trimethyl-2*H*-1-benzopyran-8-yl)-2-methyl-1-propanone, D-70348
Hypocretenoic acid; Me ester, *in* H-70235
Methyl yomoginate, *in* H-70199

$C_{16}H_{20}O_5$
Curvularin, C-80166
Evodione, E-80091
Glutinopallal, G-70021

$C_{16}H_{20}O_6$
11α-Hydroxycurvularin, *in* C-80166
11β-Hydroxycurvularin, *in* C-80166
Orthopappolide, O-60045
▷ Pyrenophorin, P-70167

$C_{16}H_{20}O_8$
Linocinnamarin, *in* H-80242

$C_{16}H_{20}O_9$
Gentiopicroside, G-80009

$C_{16}H_{21}BrO_4$
1-(4-Bromo-2,5-dihydroxyphenyl)-7-hydroxy-3,7-dimethyl-2-octen-1-one, B-70206

$C_{16}H_{22}$
[3^{4,10}][7]Metacyclophane, M-60030

$C_{16}H_{22}ClN_3O$
Folicur, F-80071

$C_{16}H_{22}O$
2,4-Bis(3-methyl-2-butenyl)phenol, B-80155
4-(1,1-Dimethyl-2-propenyl)-2-(3-methyl-2-butenyl)phenol, D-80471
6,8,12,14-Hexadecatetraen-10-yn-1-ol, H-80041

$C_{16}H_{22}O_2$
6-Methoxyprimnatrienone, *in* P-80174

$C_{16}H_{22}O_3$
3α-Hydroxydesoxoachalensolide; 3-Me ether, *in* H-70135
3β-Hydroxydesoxoachalensolide; Me ether, *in* H-70135
2-(3-Hydroxy-3,7-dimethyl-2,6-octadienyl)-1,4-benzenediol, *in* H-80153
3-Hydroxy-1,4(15),11(13)-eudesmatrien-12-oic acid; Me ester, *in* H-80164
3-Hydroxy-6-methoxyprimnatrienone, *in* P-80174
7-Octynoic acid; Anhydride, *in* O-80024

$C_{16}H_{22}O_5$
ent-7β-Hydroxy-13,14,15,16-tetranor-3-cleroden-12-oic acid 18,19-lactone, H-70226
Methyl altamisate, *in* A-70084

$C_{16}H_{22}O_6$
2α,3α-Epoxy-1β,4α-dihydroxy-8β-methoxy-7(11)-eudesmen-12,8-olide, *in* E-60033

$C_{16}H_{22}O_6S_3$
2,8,17-Trithia[4^{5,12}][9]metacyclophane; Trisulfone, *in* T-70328

$C_{16}H_{22}O_8$
Synrotolide, S-60066

$C_{16}H_{22}O_{10}$
Gelsemide 7-glucoside, *in* G-60010

$C_{16}H_{22}O_{11}$
myo-Inositol; 1,2,3,4,6-Penta-Ac, *in* I-80015

$C_{16}H_{22}S_3$
2,8,17-Trithia[4^{5,12}][9]metacyclophane, T-70328

$C_{16}H_{23}N$
Axisonitrile-4, *in* A-60328

$C_{16}H_{23}NO$
2-(Aminomethyl)cyclooctanol; *N*-Benzoyl, *in* A-70170

$C_{16}H_{23}NO_2$
2-Amino-4-*tert*-butylcyclopentanol; Benzoyl, *in* A-70104

$C_{16}H_{23}NS$
Axisothiocyanate-4, *in* A-60329

$C_{16}H_{23}N_3OS$
▷ Buprofezin, B-80276

$C_{16}H_{23}N_5O_5$
1′-Methylzeatin; 9-β-D-Ribofuranosyl, *in* M-60133

$C_{16}H_{24}$
Pentacyclo[11.3.0.0^{1,5}.0^{5,9}.0^{9,13}]hexadecane, P-70020

$C_{16}H_{24}O$
7,9,11,13-Hexadecatetraen-1-al, H-80040
7,12,14-Hexadecatrien-10-yn-1-ol, H-80044
5-Methyl-2-(1-methyl-1-phenylethyl)cyclohexanol, M-60090

$C_{16}H_{24}O_2$
4-Methoxy-1,9-cadinadien-3-one, *in* H-80136

$C_{16}H_{24}O_3$
2-(3-Hydroxy-3,7-dimethyl-6-octenyl)-1,4-benzenediol, H-80153

$C_{16}H_{24}O_4$
Furodysinin hydroperoxide, F-70054
1-Isobutyryloxymethyl-4-isopropyl-2,5-dimethoxybenzene, *in* D-70309

$C_{16}H_{24}O_4S_2$
Dithiatopazine, D-70508

$C_{16}H_{24}O_9$
Semperoside, S-60021

$C_{16}H_{24}O_{10}$
Adoxosidic acid, A-70068
1,4-Di-*O*-methyl-*myo*-inositol; Tetra-Ac, *in* D-80452
9-Hydroxysemperoside, *in* S-60021
Methylcatalpol, *in* C-70026
Vebraside, V-60003

$C_{16}H_{24}O_{11}$
Shanzhiside, S-60028

$C_{16}H_{25}GdN_4O_8$
Gadoteric acid, *in* T-60015

$C_{16}H_{25}N$
Axisonitrile-1, *in* A-60328
Axisonitrile-2, *in* A-60328
Axisonitrile-3, *in* A-60328
10α-Isocyanoalloaromadendrane, *in* A-60328
3-Isocyano-7,9-bisaboladiene, I-60091
7-Isocyano-3,10-bisaboladiene, I-60092
11-Isocyano-5-eudesmene, *in* F-60068
6-Isocyano-4(15)-eudesmene, *in* F-60069

$C_{16}H_{25}NO$
7-Isocyanato-2,10-bisaboladiene, I-60089

$C_{16}H_{25}NO_5$
Wasabidienone *E*, W-60003
Wasabidienone *E*, *in* W-70002

$C_{16}H_{25}NS$
Axisothiocyanate-1, *in* A-60329
Axisothiocyanate-2, *in* A-60329
Axisothiocyanate-3, *in* A-60329
10α-Isothiocyanatoalloaromadendrane, *in* A-60329
1-Isothiocyanato-4-cadinene, I-80094
11-Isothiocyano-5-eudesmene, *in* F-60068

$C_{16}H_{26}$
3,4,7,11-Tetramethyl-1,3,6,10-dodectetraene, T-70135

$C_{16}H_{26}O_2$
6-Isopropenyl-3-methyl-3,9-decadien-1-ol acetate, *in* I-70089
Norambreinolide, N-80075
Senecrassidiol; 5-Deoxy, 6-oxo, 8-Me ether, *in* S-80026
3,7,11-Trimethyl-2,6,10-dodecatrienoic acid; Me ester, *in* T-60364

$C_{16}H_{26}O_3$
3α-Hydroxynorambreinolide, *in* N-80075
6-Hydroxy-2,4,8-tetradecatrienoic acid; Et ester, *in* H-70222
ent-12-Hydroxy-13,14,15,16-tetranor-1(10)-halimen-18-oic acid, H-60231
Juvenile hormone III, *in* T-60364
Methylzedoarondiol, *in* Z-70004

$C_{16}H_{26}O_5$
2,3,4,6,7,8-Hexahydro-4,8-dihydroxy-2-(1-hydroxyheptyl)-5*H*-1-benzopyran-5-one, H-80057

$C_{16}H_{26}O_8$
Nepetaside, N-70031

$C_{16}H_{26}O_9$
Gelsemiol 1-glucoside, *in* G-60011
Gelsemiol 3-glucoside, *in* G-60011
Gibboside, G-60020

$C_{16}H_{27}NO$
Axamide-1, A-70272
Axamide-2, A-60327
10α-Formamidoalloaromadendrane, *in* A-60327
11-Formamido-5-eudesmene, F-60068
6-Formamido-4(15)-eudesmene, F-60069

$C_{16}H_{27}NO_8$
4-(2-Carboxyethyl)-4-nitroheptanedioic acid; Tri-Et ester, *in* C-80025

$C_{16}H_{28}N_2$
2,4,6-Tri-*tert*-butylpyrimidine, T-80219

$C_{16}H_{28}N_4O_8$
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid, T-60015

$C_{16}H_{28}O$
Dodecahydro-3*a*,6,6,9*a*-tetramethylnaphtho[2,1-*b*]furan, D-70533
11,13-Hexadecadienal, H-70033

$C_{16}H_{28}O_2$
Isoambrettolide, I-60086
6-Isopropenyl-3-methyl-9-decen-1-ol; Ac, *in* I-70089
6α-Methoxy-4(15)-eudesmen-1β-ol, *in* E-80084

$C_{16}H_{28}O_4$
3,8-Dihydroxy-13,14,15,16-tetranor-12-labdanoic acid, D-80387
Secoisolancifolide, S-80014

$C_{16}H_{28}O_7$
Betulalbuside *A*, *in* D-80456
Betulalbuside *B*, *in* D-80456

$C_{16}H_{30}$
5-Hexadecyne, H-60037

$C_{16}H_{30}N_4O_2$
Tetrahydroimidazo[4,5-*d*]imidazole-2,5(1*H*,3*H*)-dione; 1,3,4,6-Tetraisopropyl, *in* T-70066

$C_{16}H_{30}O$
Decamethylcyclohexanone, D-60011
2-Hexadecenal, H-60036
7-Hexadecenal, H-70035

$C_{16}H_{30}O_2$
8,9-Hexadecanedione, H-70034
15-Hexadecanolide, *in* H-80173
5-Hexadecenoic acid, H-80045

$C_{16}H_{32}N_2O_5$
4,7,13,16,21-Pentaoxa-1,10-diazabicyclo[8.8.5]tricosane, P-60060

$C_{16}H_{32}N_6$
Pentakis(dimethylamino)aniline, *in* B-80014

$C_{16}H_{32}O_3$
11-Hydroxyhexadecanoic acid, H-80172
15-Hydroxyhexadecanoic acid, H-80173

$C_{16}H_{34}N_4$
Octahydroimidazo[4,5-*d*]imidazole; 1,3,4,6-Tetraisopropyl, *in* O-70015

$C_{16}H_{35}NO_3$
2-Amino-1,3,4-hexadecanetriol, A-80079

$C_{16}H_{36}BF_4N$
Tetrabutylammonium(1+); Tetrafluoroborate, *in* T-80014

$C_{16}H_{36}BrNO_4$
Tetrabutylammonium(1+); Bromide, *in* T-80014

$C_{16}H_{36}ClCrNO_3$
TBACC, *in* T-80014

$C_{16}H_{36}ClNO_4$
Tetrabutylammonium(1+); Perchlorate, *in* T-80014

$C_{16}H_{36}Cl_4IN$
Tetrabutylammonium(1+); Iodotetrachloride, *in* T-80014

$C_{16}H_{36}FN$
Tetrabutylammonium(1+); Fluoride, *in* T-80014

$C_{16}H_{36}N^{\oplus}$
Tetrabutylammonium(1+), T-80014

$C_{16}H_{36}N_4$
Tetrabutylammonium(1+); Azide, *in* T-80014

$C_{16}H_{37}F_2N$
Tetrabutylammonium(1+); Bifluoride, *in* T-80014

$C_{16}H_{37}NO$
▷ Tetrabutylammonium(1+); Hydroxide, *in* T-80014

$C_{16}H_{38}N_6$
1,4,7,12,15,18-Hexaazacyclodocosane, H-70028

$C_{16}H_{38}N_6O_2$
1,13-Dioxa-4,7,10,16,19,22-hexaazacyclotetracosane, D-70460

$C_{16}H_{40}BN$
Tetrabutylammonium(1+); Borohydride, *in* T-80014

$C_{17}H_8N_2O$
10-(Dicyanomethylene)anthrone, D-60164

$C_{17}H_8OS_8$
Tetrakis(1,3-dithiol-2-ylidene)cyclopentanone, T-80131

$C_{17}H_9ClO$
10-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70047
11-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70048
2-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70040
3-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70041
4-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70042
5-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70043
6-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70044
8-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70045
9-Chloro-7*H*-benz[*de*]anthracen-7-one, C-70046

$C_{17}H_{10}F_3NO_3$
7-Amino-4-(trifluoromethyl)-2*H*-1-benzopyran-2-one; *N*-Benzoyl, *in* A-60265

$C_{17}H_{10}N_2$
1-(Diazomethyl)pyrene, D-70062
9-(Dicyanomethyl)anthracene, D-60163

$C_{17}H_{10}N_4$
Naphtho[2′,1′:5,6][1,2,4]triazino[4,3-*b*]indazole, N-80010

$C_{17}H_{10}N_4O_3S_2$
3,3′-Carbonylbis[5-phenyl-1,3,4-oxadiazole-2(3*H*)-thione], C-80021

$C_{17}H_{10}O$
3*H*-Cyclonona[*def*]biphenylen-3-one, C-70230

$C_{17}H_{10}O_2$
2*H*-Anthra[1,2-*b*]pyran-2-one, A-80164
3*H*-Anthra[2,1-*b*]pyran-3-one, A-80165

$C_{17}H_{10}O_4$
Fluorescamine, F-80017
Neorauteen, *in* N-80020

$C_{17}H_{10}O_5$
1,5-Diphenylpentanepentone, D-60488

$C_{17}H_{10}O_7$
2-Hydroxy-3-methoxy-8,9-methylenedioxycoumestan, *in* T-80088
3-Hydroxy-2-methoxy-8,9-methylenedioxycoumestan, *in* T-80088
3-Hydroxy-4-methoxy-8,9-methylenedioxycoumestan, *in* T-80089

$C_{17}H_{10}O_8$
Scapaniapyrone *A*, S-70017

$C_{17}H_{11}N$
Dibenzo[*f*,*h*]quinoline, D-70075

$C_{17}H_{11}NO$
Benz[*cd*]indol-2-(1*H*)-one; *N*-Ph, *in* B-70027

$C_{17}H_{11}NO_2$
11*H*-Benzo[*a*]carbazole-1-carboxylic acid, B-80017

$C_{17}H_{11}N_3$
7,12-Dihydropyrido[3,2-*b*:5,4-*b*′]diindole, D-70254
7,12-Dihydropyrido[3,2-*b*:5,4-*b*′]diindole, D-80246

$C_{17}H_{12}$
3*H*-Cyclonona[*def*]biphenylene, C-60215
Cycloocta[*def*]fluorene, C-70233
1*H*-Cyclopenta[*l*]phenanthrene, C-80190
1-Methylazupyrene, M-60043

$C_{17}H_{12}BrN$
Dibenzo[*a*,*h*]quinolizinium(1+); Bromide, *in* D-70076
Naphtho[1,2-*a*]quinolizinium(1+); Bromide, *in* N-70012

$C_{17}H_{12}ClNO_4$
Dibenzo[*a*,*h*]quinolizinium(1+); Perchlorate, *in* D-70076
Naphtho[1,2-*a*]quinolizinium(1+); Perchlorate, *in* N-70012

$C_{17}H_{12}Cl_2O_8$
Geodoxin, G-70007

$C_{17}H_{12}N^{\oplus}$
Dibenzo[*a*,*h*]quinolizinium(1+), D-70076
Naphtho[1,2-*a*]quinolizinium(1+), N-70012

$C_{17}H_{12}N_2$
2-Phenylpyrimido[2,1,6-*de*]quinolizine, P-80131

$C_{17}H_{12}N_2O$
2-Benzoyl-1,2-dihydro-1-isoquinolinecarbonitrile, B-70073

$C_{17}H_{12}OS$
2,6-Diphenyl-4*H*-thiopyran-4-one, D-60492

$C_{17}H_{12}O_2$
5,11-Methanodibenzo[*a*,*e*]cyclooctene-6,12(5*H*,11*H*)dione, M-80040
2,2′-Spirobi[2*H*-1-benzopyran], S-70062

$C_{17}H_{12}O_3$
1,2-Diphenyl-1,2-cyclopropanedicarboxylic acid; Anhydride, *in* D-80509
1-(4-Hydroxy-5-benzofuranyl)-3-phenyl-2-propen-1-one, H-70107
Salvinolactone, S-80006

$C_{17}H_{12}O_3S$
2,6-Diphenyl-4*H*-thiopyran-4-one; 1,1-Dioxide, *in* D-60492
5-Methoxy-2-(phenylthio)-1,4-naphthoquinone, *in* H-70213
5-Methoxy-3-(phenylthio)-1,4-naphthoquinone, *in* H-70214

$C_{17}H_{12}O_4$
Neodunol, N-80020

$C_{17}H_{12}O_5$
5-Methoxy-6,7-methylenedioxyflavone, *in* T-60322
7-Methoxy-3′,4′-methylenedioxyisoflavone, *in* H-80203

$C_{17}H_{12}O_6$
3,3-Dihydroxy-5,5-diphenyl-1,2,4,5-pentanetetrone, *in* D-60488
4-(3,4-Dihydroxyphenyl)-6,7-dihydroxy-2-naphthalenecarboxylic acid, D-80358
3-Hydroxy-7,9-dimethoxycoumestan, *in* T-80294
3-Hydroxy-8,9-dimethoxycoumestan, *in* T-80295
2′-Hydroxy-5-methoxy-6,7-methylenedioxyisoflavone, *in* T-80108
4′-Hydroxy-5-methoxy-6,7-methylenedioxyisoflavone, *in* D-80341
5-Hydroxy-2′-methoxy-6,7-methylenedioxyisoflavone, *in* T-60107
7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavone, *in* T-80107
7-Hydroxy-6-methoxy-3′,4′-methylenedioxyisoflavone, *in* T-80111
7-Hydroxy-8-methoxy-3′,4′-methylenedioxyisoflavone, *in* T-70112
3-Hydroxy-4-methoxy-8,9-methylenedioxypterocarpene, *in* T-80122

$C_{17}H_{12}O_7$
3,8-Dihydroxy-6-methoxy-1-methylanthraquinone-2-carboxylic acid, *in* T-80323

5,7-Dihydroxy-6-methoxy-3′,4′-methylenedioxyisoflavone, *in* P-80043
6*a*-Hydroxy-3,4:8,9-bis(methylenedioxy)pterocarpan, *in* P-80053
3,6,8-Trihydroxy-1-methylanthraquinone-2-carboxylic acid; Me ester, *in* T-60332

$C_{17}H_{12}O_8$
Nasutin *B*, *in* E-70007

$C_{17}H_{13}BF_4N_2$
Urorosein; Tetrafluoroborate, *in* U-80033

$C_{17}H_{13}BrN_2$
Urorosein; Bromide, *in* U-80033

$C_{17}H_{13}ClN_2$
Urorosein; Chloride, *in* U-80033

$C_{17}H_{13}ClN_2O_4$
Urorosein; Perchlorate, *in* U-80033

$C_{17}H_{13}NO_2S$
2-Phenyl-1,5-benzothiazepin-4(5*H*)-one; *N*-Ac, *in* P-60081

$C_{17}H_{13}NO_4$
2-Oxo-3-indolineglyoxylic acid; Benzyl ester, *in* O-80085

$C_{17}H_{13}NS$
1-Methyl-4-phenyl-1λ^4-1-benzothiopyran-2-carbonitrile, M-80142

$C_{17}H_{13}N_2^{\oplus}$
Urorosein, U-80033

$C_{17}H_{13}N_3$
1-Anilino-γ-carboline, *in* A-70114

$C_{17}H_{14}$
2,3-Dihydro-1*H*-cyclopenta[*l*]phenanthrene, D-80177
6,12-Methanobenzocyclododecene, M-80039

$C_{17}H_{14}ClF_7O_2$
Tefluthrin, T-80004

$C_{17}H_{14}Cl_2O_7$
Tumidulin, T-70334

$C_{17}H_{14}N_2$
3,3′-Methylenebisindole, M-80078

$C_{17}H_{14}N_2O_4$
2,3-Dihydro-2-hydroxy-1*H*-imidazole-4,5-dione; 1,3-Di-Ph, *O*-Ac, *in* D-60243

$C_{17}H_{14}O$
2-Methoxy-1-phenylnaphthalene, *in* P-60115
2-Methoxy-5-phenylnaphthalene, *in* P-60118
7-Methoxy-1-phenylnaphthalene, *in* P-60119

$C_{17}H_{14}O_2$
1,2-Dihydro-1-phenyl-1-naphthalenecarboxylic acid, D-60264
2-(4-Hydroxyphenyl)-5-(1-propenyl)benzofuran, H-60214
9-Phenanthreneacetic acid; Me ester, *in* P-70047
9-Phenanthrenemethanol; Ac, *in* P-80079
2-(Phenylethynyl)benzoic acid; Et ester, *in* P-70074

$C_{17}H_{14}O_3$
1,5-Diphenyl-1,3,5-pentanetrione, D-60489
7-Methoxy-2-methylisoflavone, *in* H-80205
1-(β-Methylcrotonoyloxy)-5-benzoyl-2,4-pentadiyne, *in* H-80235
4-[5-(1-Propenyl)-2-benzofuranyl]-2,3-benzenediol, *in* H-60214

$C_{17}H_{14}O_4$
1-Acetoxy-7-(3-acetoxyphenyl)-2-heptene-4,6-diyne, *in* H-80234
Agrostophyllin, A-70077
Bonducellin, B-60192
9,10-Dimethoxy-2-methyl-1,4-anthraquinone, D-80413
3,9-Dimethoxypterocarpene, *in* D-80376
1,2-Diphenyl-1,2-cyclopropanedicarboxylic acid, D-80509

$C_{17}H_{14}O_4S$
2-(1,3-Pentadiynyl)-5-(3,4-diacetoxy-1-butynyl)thiophene, *in* P-80025

$C_{17}H_{14}O_5$
Benzophenone-2,2′-dicarboxylic acid; Di-Me ester, *in* B-70041
▷ 1,3-Dihydroxy-2-(ethoxymethyl)anthraquinone, *in* D-70306
2′,5-Dihydroxy-7-methoxyflavone, *in* T-80299
4′-Hydroxy-3′,7-dimethoxyflavone, *in* T-80308
5-Hydroxy-6,7-dimethoxyflavone, *in* T-60322
6-Hydroxy-4′,7-dimethoxyisoflavone, *in* T-80310
7-Hydroxy-3′,4′-dimethoxyisoflavone, *in* T-80308
7-Hydroxy-4′,5-dimethoxyisoflavone, *in* T-80309
7-Hydroxy-4′,8-dimethoxyisoflavone, *in* T-80311
3-Hydroxy-1-methoxy-2-(methoxymethyl)anthraquinone, *in* D-70306
2-(2-Hydroxy-4-methoxyphenyl)-3-methyl-5,6-methylenedioxybenzofuran, H-70157
Intricatinol, I-80017
Pterocarpin, *in* M-70001
Puerol *A*, P-70137
3,6,7-Trimethoxy-1,4-phenanthraquinone, T-80348

$C_{17}H_{14}O_6$
4′,5-Dihydroxy-3′,7-dimethoxyflavone, D-70291
3,4′-Dihydroxy-6,7-dimethoxyflavone, *in* T-80092
3′,7-Dihydroxy-4′,6-dimethoxyflavone, *in* T-80092
4′,7-Dihydroxy-3,6-dimethoxyflavone, *in* T-80092
2′,5-Dihydroxy-7,8-dimethoxyisoflavone, *in* T-70110
3′,7-Dihydroxy-4′,6-dimethoxyisoflavone, *in* T-80111
4′,5-Dihydroxy-3′,7-dimethoxyisoflavone, *in* T-80109
4′,5-Dihydroxy-6,7-dimethoxyisoflavone, *in* T-80112
4′-6-Dihydroxy-5,7-dimethoxyisoflavone, *in* T-80112
4′,7-Dihydroxy-2′,5-dimethoxyisoflavone, *in* T-80106
5,7-Dihydroxy-2′,4′-dimethoxyisoflavone, *in* T-80106
5,7-Dihydroxy-2′,6-dimethoxyisoflavone, *in* T-60107
5,7-Dihydroxy-3′,4′-dimethoxyisoflavone, *in* T-80109
5,7-Dihydroxy-4′,6-dimethoxyisoflavone, *in* T-80112
5-Hydroxy-4-(3-hydroxy-4-methoxyphenyl)-7-methoxycoumarin, *in* D-80356
7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavanone, *in* T-80101
2-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan, *in* T-80117
3-Hydroxy-4-methoxy-8,9-methylenedioxypterocarpan, *in* T-80119
4-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan, *in* T-80119
Sophorocarpan *B*, S-60038

$C_{17}H_{14}O_7$
Arizonin A_1, *in* A-70254
Arizonin B_1, *in* A-70254
6*a*,12*a*-Dihydro-3,4,10-trihydroxy-8-methoxy[2]benzopyrano[4,3-*b*][1]benzopyran-7(5*H*)-one, *in* C-70200
6*a*,12*a*-Dihydro-2,3,10-trihydroxy-8-methoxy[2]benzopyrano[4,3-*b*][1]benzopyran-7(5*H*)-one, 9CI, *in* C-70200
1,3-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan, *in* P-80051
4-(3,4-Dihydroxyphenyl)-8-hydroxy-5,7-dimethoxycoumarin, *in* D-80370
Irispurinol, I-80044
Nornotatic acid, *in* N-70081
3′,5,7-Trihydoxy-4′,6-dimethoxyisoflavone, *in* P-80043
2′,5,7-Trihydroxy-4′,5′-dimethoxyflavone, *in* P-80033
3,4′,5-Trihydroxy-6,7-dimethoxyflavone, *in* P-80035
3,4′,7-Trihydroxy-5,6-dimethoxyflavone, *in* P-80035
3′,4′,5-Trihydroxy-6,7-dimethoxyisoflavone, *in* P-70032
3′,5,7-Trihydroxy-4′,8-dimethoxyisoflavone, *in* P-80045
4′,5,7-Trihydroxy-3′,6-dimethoxyisoflavone, *in* P-80043
4′,5,7-Trihydroxy-3′,8-dimethoxyisoflavone, *in* P-80045

$C_{17}H_{14}O_8$
3′,4′,5,5′-Tetrahydroxy-6,7-dimethoxyflavone, *in* H-70081
3′,4′,5,7-Tetrahydroxy-5′,6-dimethoxyflavone, *in* H-70081
4′,5,6,7-Tetrahydroxy-3,3′-dimethoxyflavone, *in* H-80067

$C_{17}H_{14}S_5$
4,5-Dimercapto-1,3-dithiole-2-thione; Dibenzyl thioether, *in* D-80409

$C_{17}H_{15}ClO_7$
Methyl 2-(3-chloro-2,6-dihydroxy-4-methylbenzoyl)-5-hydroxy-3-methoxybenzoate, *in* S-70083

$C_{17}H_{15}N$
2-Methyl-1,5-diphenyl-1*H*-pyrrole, *in* M-60115

$C_{17}H_{15}NO_2S$
2-Phenyl-1,5-benzothiazepin-4(5*H*)-one; 2,3-Dihydro, *N*-Ac, *in* P-60081

$C_{17}H_{16}$
1,1-Diphenyl-1,3-pentadiene, D-70489

$C_{17}H_{16}N_2O$
1-[1-Methoxy-1-(2-pyridinyl)ethyl]isoquinoline, *in* I-60134

$C_{17}H_{16}N_2O_2$
3,5-Pyrazolidinedione; 1,2-Dibenzyl, *in* P-80200

$C_{17}H_{16}N_2O_3$
3-Oxopentanedioic acid; Dianilide, *in* O-60084

$C_{17}H_{16}O_2$
1,5-Bis(4-hydroxyphenyl)-1,4-pentadiene, B-60162
5,5-Diphenyl-4-pentenoic acid, D-80513
3,3′,4,4′-Tetrahydro-2,2′-spirobi[2*H*-1-benzopyran], T-70094

$C_{17}H_{16}O_3$
Danshenspiroketallactone, D-70004
Epidanshenspiroketallactone, *in* D-70004
2,3,7-Trimethoxyphenanthrene, *in* T-60339
2,4,7-Trimethoxyphenanthrene, *in* P-80080

$C_{17}H_{16}O_4$
Cryptoresinol, C-70201
1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80139
10-Hydroxy-11-methoxydracaenone, *in* D-70546
2-(2-Hydroxy-4-methoxyphenyl)-6-methoxy-3-methylbenzofuran, H-70156
3,11-Tridecadiene-5,7,9-triyne-1,2-diol; Di-Ac, *in* T-80254
3,5,7-Trimethoxy-2-phenanthrenol, *in* T-60120

$C_{17}H_{16}O_4S_2$
5-(3,4-Diacetoxy-1-butynyl)-5′-methyl-2,2′-bithiophene, *in* M-70054

$C_{17}H_{16}O_5$
Comaparvin, C-70191
Combretastatin A2, *in* D-80360
2′,7-Dihydroxy-4′,8-dimethoxyisoflavene, *in* T-80104
3′,7-Dihydroxy-2′,4′-dimethoxyisoflavene, *in* T-80103
4′,7-Dihydroxy-2′,3′-dimethoxyisoflavene, *in* T-80103

7,10-Dihydroxy-11-methoxydracaenone, *in* D-70546
1-(2,4-Dihydroxy-3-methoxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one, *in* H-80245
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one, *in* H-80246
5,10-Dihydroxy-8-methoxy-2-propyl-4*H*-*naphtho*[1,2-*b*]pyran-4-one, 9CI, *in* C-70191
7,9-Dihydroxy-2,3,4-trimethoxyphenanthrene, *in* P-70035
Fruscinol acetate, *in* F-80084
5-Hydroxy-7,8-dimethoxyflavone, *in* T-60321
2′-Hydroxy-4′,7-dimethoxyisoflavanone, *in* T-80303
7-Hydroxy-2′,4′-dimethoxyisoflavanone, *in* T-80303
6*a*-Hydroxy-3,9-dimethoxypterocarpan, *in* T-80337
3-Hydroxy-2,9-dimethoxypterocarpan, *in* T-80335
3-Hydroxy-4,9-dimethoxypterocarpan, *in* T-80336
3-Hydroxy-9,10-dimethoxypterocarpan, *in* T-80338
4-Hydroxy-3,9-dimethoxypterocarpan, *in* T-80336
9-Hydroxy-2,3-dimethoxypterocarpan, *in* T-80335
7-Hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavan, *in* T-80097
Methylsainfuran, *in* S-60002
Sophorocarpan *A*, S-60037
1,5,6-Trimethoxy-2,7-phenanthrenediol, *in* P-60050
1,5,7-Trimethoxy-2,6-phenanthrenediol, *in* P-60050

$C_{17}H_{16}O_6$
Anhydrobyakangelicin, *in* B-80296
1,5-Bis(3,4-dihydroxyphenyl)-4-pentyne-1,2-diol, B-60155
4′,5-Dihydroxy-2′,7-dimethoxyflavanone, *in* T-80100
5,7-Dihydroxy-2′,8-dimethoxyflavanone, *in* T-70104
3′,7-Dihydroxy-2′,4′-dimethoxyisoflavanone, *in* T-80099
4′,7-Dihydroxy-2′,3′-dimethoxyisoflavanone, *in* T-80099
5,7-Dihydroxy-2′,4′-dimethoxyisoflavanone, *in* T-80100
2,10-Dihydroxy-3,9-dimethoxypterocarpan, *in* T-80118
5,8-Dihydroxy-2,3,6-trimethyl-1,4-naphthoquinone; Di-Ac, *in* D-60380
Neobyakangelicol, *in* B-80296
Olivin, O-80043
Ougenin, O-80050
Pendulone, P-80018
2′,3′,4′,6,7-Pentahydroxyisoflavene; 2′,4′ or 3′,4′-Di-Me ether, *in* P-80040
1,2,3,4-Tetramethoxyxanthone, *in* T-60126
1,3,5,8-Tetramethoxyxanthone, *in* T-70123

$C_{17}H_{16}O_7$
Isosulochrin, *in* S-70083
Sulochrin, S-70083
2′,3,5-Trihydroxy-7,8-dimethoxyflavanone, *in* P-60045
4′,5,7-Trihydroxy-3′,6-dimethoxyflavanone, *in* P-70028
4′,5,7-Trihydroxy-2′,3′-dimethoxyisoflavanone, *in* P-80039
1,3,8-Trihydroxy-4,7-dimethoxyxanthone, *in* P-60052

$C_{17}H_{17}ClO_6$
Byakangelicin; 3′-Deoxy, 3′-chloro, *in* B-80296

$C_{17}H_{17}NO$
5,6,11,12-Tetrahydrodibenz[*b,f*]azocine; *N*-Ac, *in* T-70057

$C_{17}H_{17}NO_2$
4-Amino-3,4-dihydro-2-phenyl-2*H*-1-benzopyran; *N*-Ac, *in* A-80067

$C_{17}H_{17}NO_4$
4-Phenyl-2,6-pyridinedicarboxylic acid; Di-Et ester, *in* P-80130

$C_{17}H_{18}O_2S_2$
3,3-Bis(phenylthio)propanoic acid; Et ester, *in* B-70157

$C_{17}H_{18}O_3$
5-Hydroxy-5,5-diphenylpentanoic acid, H-80155

$C_{17}H_{18}O_4$
Anisocoumarin A, A-80159
3′,5-Dimethoxy-3,4-methylenedioxybibenzyl, *in* T-60102
3-(2,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* D-80366
4′-Hydroxy-3′,7-dimethoxyflavan, *in* T-70260
2′-Hydroxy-4′,7-dimethoxyisoflavan, *in* T-80302
4′-Hydroxy-2′,7-dimethoxyisoflavan, *in* T-80302
7-Hydroxy-2′,4′-dimethoxyisoflavan, *in* T-80302
2-*O*-Methylangolensin, *in* A-80155
4-*O*-Methylangolensin, *in* A-80155
Pygmaeoherin, P-70145
1-(2,4,6-Trimethoxyphenyl)-3-phenyl-1-propanone, *in* T-80332

$C_{17}H_{18}O_5$
9β-Acetoxy-3-oxo-1,4(15),11(13)-eudesmatrien-12,6-olide, *in* H-60202
Combretastatin A3, *in* D-80360
11,13-Dehydromatricarin, *in* M-80010
9,10-Dihydro-2,7-dihydroxy-3,4,6-trimethoxyphenanthrene, *in* D-70246
9,10-Dihydro-5,6-dihydroxy-1,3,4-trimethoxyphenanthrene, *in* P-70034
9,10-Dihydro-5,6,7-trimethoxy-2,3-phenanthrenediol, *in* D-70246
5,7-Dihydroxy-3′,4′-dimethoxyflavan, *in* T-60103
2′,4′-Dihydroxy-5,7-dimethoxyisoflavan, *in* T-80096
2′,7-Dihydroxy-3′,4′-dimethoxyisoflavan, *in* T-80095
2′,7-Dihydroxy-4′,5-dimethoxyisoflavan, *in* T-80096
2′,7-Dihydroxy-4′,6-dimethoxyisoflavan, *in* T-80098
4′-Hydroxy-3′,5-dimethoxy-3,4-methylenedioxybibenzyl, *in* P-60044
4-(2-Hydroxy-4,6-dimethoxyphenyl)-1-(4-hydroxyphenyl)-1-propanone, *in* H-80243
Isomurralonginol; Ac, *in* I-70071
Longipesin; 9-Ac, *in* L-60034

$C_{17}H_{18}O_6$
Antibiotic L 660631, A-70224
3-(3,4-Dihydroxybenzyl)-3,7-dihydroxy-4-methoxychroman, *in* D-70288
Epicatechin; $O^{3'}$,$O^{4'}$-Di-Me, *in* P-70026
Epicatechin; $O^{3'}$,O^{5}-Di-Me, *in* P-70026
Pandoxide, P-60002
3,3′,5-Trihydroxy-4′,7-dihydroxyflavan, *in* P-70026
3′,7,8-Trihydroxy-2′,4′-dimethoxyisoflavan, *in* P-80038

$C_{17}H_{18}O_7$
Byakangelicin, B-80296
Fusarubin; O^3-Et, *in* F-60108
Fusarubin ethyl acetal, *in* F-60108
Isobyakangelicolic acid, I-80051

$C_{17}H_{18}O_9$
Furocoumarinic acid; *O*-β-D-Glucopyranoside, *in* H-80113

$C_{17}H_{19}N$
2,3,4,5-Tetrahydro-1*H*-1-benzazepine; *N*-Benzyl, *in* T-70036

$C_{17}H_{19}NO_3$
3,4,6-Trimethoxy-1,2-dimethylcarbazole, *in* T-70253

$C_{17}H_{20}$
1,7,9,15-Heptadecatetraene-11,13-diyne, H-80019

$C_{17}H_{20}N_2$
1-Ethyl-2,3,4,6,7,12-hexahydroindolo[2,3-*a*]quinolizine, E-80064

$C_{17}H_{20}N_2O$
▷ *N,N′*-Diethyl-*N,N′*-diphenylurea, *in* D-70499

$C_{17}H_{20}O$
15,16-Dihydro-17*H*-cyclopenta[*a*]phenanthren-17-one, D-80178

$C_{17}H_{20}O_2$
1,5-Diphenyl-1,3-pentanediol, D-70490

$C_{17}H_{20}O_3$
1β-Acetoxy-4(15),7(11),8-eudesmatrien-12,8-olide, *in* H-60141
15-Acetoxytubipofuran, *in* T-70332

$C_{17}H_{20}O_4$
1β-Acetoxy-3,7(11),8-eudesmatrien-12,8-olide, *in* H-60140
12,13-Dihydroxy-8,11,13-podocarpatriene-3,7-dione, D-80374
1-(2-Hydroxy-4-methoxyphenyl)-3-(3-hydroxy-4-methoxyphenyl)propane, *in* D-70336
1-(4-Hydroxy-2-methoxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)propane, *in* D-70336
1-(2-Hydroxy-4-methoxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)propene, *in* D-70336
Zaluzanin *D*, *in* Z-60001

$C_{17}H_{20}O_5$
6-Acetylferulidin, *in* F-70006
Cavoxinine, C-60024
Cavoxinone, C-60025
1-(3,4-Dihydroxyphenyl)-2-(3,4,5-trimethoxyphenyl)ethane, *in* D-80371
3,5-Dihydroxy-3′,4,4′-trimethoxybibenzyl, *in* D-80360
4,4′-Dihydroxy-3,3′,5-trimethoxybibenzyl, *in* D-80360
4,4′-Dihydroxy-3,3′,5-trimethoxybibenzyl, *in* P-60044
8-Hydroxyachillin; Ac, *in* H-60100
Matricarin, M-80010
Murraxocin, M-60151

$C_{17}H_{20}O_6$
Achillolide *A*, *in* A-60061
1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol, B-80150
Murrayanone, M-70160
Tarchonanthus lactone, T-60009

$C_{17}H_{20}O_7$
7-Hydroxy-6-[2-hydroxy-2-(tetrahydro-2-methyl-5-oxo-2-furyl)ethyl]-5-methoxy-4-methylphthalide,8CI, H-80175
Isoapressin, I-70061

$C_{17}H_{20}O_9$
3-*O*-*Feruloylquinic acid*, *in* C-70005
4,7-Dihydroxy-5-methyl-2*H*-1-benzopyran-2-one; 4-Me ether, 7-*O*-β-D-glucopyranoside, *in* D-60348

$C_{17}H_{20}O_{10}$
Tomenin, *in* T-80287

$C_{17}H_{21}ClO_6$
Arctodecurrolide, *in* D-60325

$C_{17}H_{21}N_3$
▷ Auramine, A-70268

$C_{17}H_{22}N_6O_6$
3′-Amino-3′-deoxyadenosine; 3′*N*-Ac, 3′*N*-Me, 2′,5′-di-Ac, *in* A-70128

$C_{17}H_{22}O$
1,9,15-Heptadecatriene-11,13-diyn-8-ol, H-80020
1,9,16-Heptadecatriene-4,6-diyn-3-ol, H-80021
2,9,16-Heptadecatriene-4,6-diyn-1-ol, H-80022
2,9,16-Heptadecatriene-4,6-diyn-8-ol, H-80023

$C_{17}H_{22}O_2$
Parvifoline; Ac, *in* P-80013

$C_{17}H_{22}O_2S$
Thiofurodysin acetate, *in* T-70178
Thiofurodysinin acetate, *in* T-70179

$C_{17}H_{22}O_3$
3-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxybenzoic acid, D-70423
8,12-Epoxy-3,7,11-eudesmatrien-1-ol; Ac, *in* E-60020
6-Hydroxy-7-methoxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran, H-80191
6-Methoxy-2-(3,7-dimethyl-2,6-octadienyl)-1,4-benzoquinone, M-60038
Nimbidiol, N-60021

$C_{17}H_{22}O_4$
2-Acetoxy-2-desoxyperezone, *in* I-70075
3β-Acetoxy-4,11(13)-eudesmadien-12,8β-olide, *in* H-60136
15-Acetoxyisoalloalantolactone, *in* I-80047
9β-Acetoxytournefortiolide, *in* H-60137
1-(5,7-Dihydroxy-2,2,6-trimethyl-2*H*-1-*benzopyran*-8-*yl*)-2-*methyl*-1-*butanone*, 9*CI*, *in* D-70348
3β-Hydroxydesoxoachalensolide; Ac, *in* H-70135
15-Hydroxy-3,10(14)-guaiadien-12,8-olide; Ac, *in* H-70136
Laurenobiolide, *in* H-70134
Subexpinnatin *C*, S-60058

$C_{17}H_{22}O_4S$
15-Acetylthioxyfurodysinin lactone, A-80030

$C_{17}H_{22}O_5$
2α-Acetoxy-8-epiivangustin, *in* I-70109
6α-Acetoxy-8-epiivangustin, *in* I-70109
1β-Acetoxy-8β-hydroxy-3,7(11)-eudesmadien-12,8-olide, *in* D-60322
3β-Acetoxy-2α-hydroxy-1(10),4,11(13)-germacratrien-12,6α-olide, *in* H-60006
3-Acetylpulverulide, *in* P-80191
Cumambrin A, *in* C-80164
Ergolide, E-60035
Naematolone, *in* N-70001

$C_{17}H_{22}O_6$
15-Acetoxy-3α-hydroperoxyalloalantolactone, *in* A-80044
Cratystyolide; 3-Ac, *in* T-70257
13-Desacetyleudesmaafraglaucolide, *in* T-70258
13-Desacetyl-1α-hydroxyafraglaucolide, *in* A-70070
13-Desacetyl-1β-hydroxyafraglaucolide, *in* A-70070
13-Desacetyl-1β-hydroxyisoafraglaucolide, *in* I-70060
Neovasinone, N-60019
Neovasinone, *in* N-70029
Omphalocarpin, O-80044

$C_{17}H_{23}Br_3O_4$
9-Acetoxy-3,10,13-tribromo-4,7:6,12-diepoxy-1-pentadecyne, *in* B-70195

$C_{17}H_{23}N_5O_7$
Queuosine, *in* Q-70004

$C_{17}H_{24}Br_2O_4$
6-Acetoxy-3,10-dibromo-4,7-epoxy-12-pentadecen-1-yne, *in* B-70217

$C_{17}H_{24}Br_2O_5$
Graciosin, G-80035

$C_{17}H_{24}O_2$
Norasperenal A, N-80076
Norasperenal B, N-80077
Norasperenal D, *in* N-80077
Panaxydol, P-80006
Tochuinyl acetate, *in* T-70202

$C_{17}H_{24}O_3$
2-[2-(Acetyloxy)ethenyl]-6,10-dimethyl-2,5,9-undecatrienal, A-70050
HM-2, H-80092
HM-3, H-80093
9-Oxogymnomitryl acetate, *in* G-70035

$C_{17}H_{24}O_4$
3β-Acetoxydrimenin, *in* D-60519
9β-Acetoxy-4,11(13)-eudesmadien-12-oic acid, *in* H-60135
6β-Acetoxy-1β-hydroxy-4,11-guaiadien-3-one, *in* G-80044
9α-Acetoxy-7β-hydroxy-2-longipinen-1-one, *in* D-80332
2-(7-Hydroxy-3,7-dimethyl-2-octenyl)-6-methoxy-1,4-benzoquinone, H-60123
Isotrichodermin, *in* E-70028
Norstrictic acid, N-70080
Sterpuric acid; 13-Hydroxy, 3,13-ethylidene acetal, *in* S-60053

$C_{17}H_{24}O_5$
3β-Acetoxy-10α-hydroxy-4,11(13)-cadinadien-12-oic acid, *in* Z-70001
Altamisin, *in* A-70084
Cinnamodial, C-70177
Dihydrocumambrin A, *in* C-80164
▷ Naematolin, N-70001
Neovasinin, N-70029
Nitrosin, N-60045
4,5-Seconeopulchell-5-ene; 2-Ac, *in* S-70025
4,5-Seconeopulchell-5-ene; 4-Ac, *in* S-70025

$C_{17}H_{24}O_6$
2α-Acetoxy-11α,13-dihydroconfertin, *in* D-60211
Blumealactone *C*, B-70172
15-Desacetyltetraneurin *C*, *in* T-60158
6β-Hydroxypulchellin 2-*O*-acetate, *in* P-80189
Naematolin *B*, *in* N-70001
Paramicholide, P-70011
Tetraneurin *D*, T-60158

$C_{17}H_{24}O_7$
8α-Acetoxy-3α,4α,10β-trihydroxy-1-guaien-12,6α-olide, *in* T-80094

$C_{17}H_{24}O_9$
Syringin, *in* S-70046

$C_{17}H_{24}O_{10}$
Pseudo-α-D-glucopyranose; Penta-Ac, *in* H-70170

$C_{17}H_{24}O_{12}$
Sesamoside, S-70036

$C_{17}H_{25}ClO_3$
1-Chloro-9,10-epoxy-4,6-heptadecadiyne-2,3-diol, *in* P-80006

$C_{17}H_{25}NO_4$
N-Acetylparthenolidine, *in* P-80012

$C_{17}H_{26}N_2O_3$
Dibusadol, *in* H-70108

$C_{17}H_{26}O$
Acetylcedrene, A-70032
8,10,12,14-Heptadecatetraen-1-al, H-80018

$C_{17}H_{26}O_2$
3-Acetoxysterpurene, *in* S-80045
Coralloidin *C*, *in* E-60066
Coralloidin *E*, *in* E-60065
Cyperenyl acetate, *in* C-70259
Dihydrotochuinyl acetate, *in* T-70202
11-Phenylundecanoic acid, P-70096
12-Sesquisabinenol acetate, *in* S-70037
13-Sesquisabinenol acetate, *in* S-70037

$C_{17}H_{26}O_3$
8,9-Dihydroxy-4,6-heptadecadiyn-3-one, D-80321
1-Heptadecene-4,6-diyne-3,9,10-triol, H-80024
9α-Hydroxygymnomitryl acetate, *in* G-70035
3-(1,3,5,7,9-Tetradecapentaenyloxy)-1,2-propanediol, T-70024

$C_{17}H_{26}O_4$
3β-Acetoxy-4,10(14)-oplopadiene-8β,9α-diol, *in* O-70042
10α-Ethoxy-3β-hydroxy-4,11(13)-cadinadien-12-oic acid, *in* Z-70001
Norhardwickiic acid, N-70077

$C_{17}H_{26}O_{10}$
Adoxoside, A-70067
Secologanol, S-80016

$C_{17}H_{26}O_{11}$
5-Deoxypulchelloside *I*, *in* P-70139
6β-Hydroxyadoxoside, *in* A-70067
Shanzhiside; Me ester, *in* S-60028

$C_{17}H_{26}O_{12}$
Pulchelloside I, P-70139

$C_{17}H_{27}N$
[12](2,6)Pyridinophane, P-80216

$C_{17}H_{27}NO_4$
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid; Di-*tert*-butyl ester, *in* D-80193

$C_{17}H_{28}O_2$
5,6-Decanediol; Benzyl ether, *in* D-60013

$C_{17}H_{28}O_3$
6β-Acetoxy-1α,4α-epoxyeudesmane, *in* E-60019
3-Acetoxy-1(10),5-germacradien-4-ol, *in* G-80010
Carotdiol acetate, *in* D-80004
Fauronyl acetate, *in* F-70002
5,10(14)-Germacradiene-1,4-diol; 1-Ac, *in* G-70009
4,6-Heptadecadiyne-3,8,9-triol, *in* D-80321

$C_{17}H_{28}O_4$
6β-Acetoxy-4(15)-eudesmene-1β,5α-diol, *in* E-60068
Shiromodiol; 8-Ac, *in* S-70039

$C_{17}H_{28}O_5$
12-Acetoxy-5,8-dihydroxyfarnesol, *in* T-60363

$C_{17}H_{29}N$
2,4,6-Tri-*tert*-butylpyridine, T-70217

$C_{17}H_{30}O$
3,4,7,11-Tetramethyl-6,10-tridecadienal, T-60156

$C_{17}H_{32}$
1,1,2,2,3,3,4,4,5,5-Decamethyl-6-methylenecyclohexane, D-60012

$C_{17}H_{32}O_2$
Cyclopentadecanone; Ethylene acetal, *in* C-60219

$C_{17}H_{32}O_4$
2-Dodecyl-3-methylbutanedioic acid, D-80527

$C_{17}H_{34}O$
6,12-Dimethyl-2-pentadecanone, D-80465
Undecamethylcyclohexanol, U-60003

$C_{17}H_{34}O_3$
11-Hydroxyhexadecanoic acid; Me ester, *in* H-80172

$C_{17}H_{36}I_2N_2$
Camphonium, *in* T-70277

$C_{17}H_{36}N_2^{2\oplus}$
Trimethidinium(2+), T-70277

$C_{17}H_{37}NO_2$
Tetrabutylammonium(1+); Formate, *in* T-80014

$C_{17}H_{37}N_3O_3$
1,7,14-Trioxa-4,11,17-triazacycloeicosane; 4,11,17-Tri-Me, *in* T-80357

$C_{18}H_6N_6O_{12}$
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tripyrazine-2,3,6,7,10,11-tetracarboxylic acid, B-60051

$C_{18}H_8N_2O_6$
1,1′-(1,2-Dioxo-1,2-ethanediyl)bis-1*H*-indole-2,3-dione, D-70466

$C_{18}H_8O_6$
10-Hydroxy-2*H*,13*H*-furo[3,2-*c*:5,4-*h*′]bis[1]benzopyran-2,13-dione, H-70133

$C_{18}H_9ClO_2$
7-Oxo-7*H*-benz[*de*]anthracene-2-carboxylic acid; Chloride, *in* O-80059
7-Oxo-7*H*-benz[*de*]anthracene-3-carboxylic acid; Chloride, *in* O-80060

$C_{18}H_9NO$
2-Cyanobenzanthrone, *in* O-80059
3-Cyanobenzanthrone, *in* O-80060
4-Cyanobenzanthrone, *in* O-80061

$C_{18}H_9N_3O_3$
19,20,21-Triazatetracyclo[13.3.1.1^{3,7}.1^{9,13}]heneicosa-1(19),3,5,7(21),9,11,13(20),15,17-nonaene-2,8,14-trione, T-60236

$C_{18}H_{10}$
▷ Cyclopenta[*cd*]pyrene, C-60223
1,8-Diethynylanthracene, D-80155

$C_{18}H_{10}N_2$
9,10-Dihydro-9,10-ethenoanthracene-11,12-dicarboxylic acid; Dinitrile, *in* D-70208

$C_{18}H_{10}N_2O_2$
Triphenodioxazine, T-60378

$C_{18}H_{10}N_6$
Quinoxalino[1″,2″:1′,2′]imidazo[4′,5′:4,5]imidazo[1,2-*a*]quinoxaline, Q-80005

$C_{18}H_{10}O$
Pyreno[4,5-*b*]furan, P-60214
Pyreno[1,2-*c*]furan, P-70165
Pyreno[4,5-*c*]furan, P-70166

$C_{18}H_{10}OS$
Triphenyleno[1,12-*bcd*]thiophene; *S*-Oxide, *in* T-70310

$C_{18}H_{10}O_2$
Benz[*a*]anthracene-1,2-dione, B-70012
Benz[*a*]anthracene-3,4-dione, B-70013
Benz[*a*]anthracene-5,6-dione, B-70014
Benz[*a*]anthracene-7,12-dione, B-70015
Benz[*a*]anthracene-8,9-dione, B-70016
Benzo[*c*]phenanthrene-3,4-dione, B-80034
Naphth[2,3-*a*]azulene-5,12-dione, N-60006
1,3-Pyrenedicarboxaldehyde, P-80202
1,2-Triphenylenedione, T-70308
1,4-Triphenylenedione, T-70309

$C_{18}H_{10}O_2S$
Triphenyleno[1,12-*bcd*]thiophene; *S*-Dioxide, *in* T-70310

$C_{18}H_{10}O_3$
7-Oxo-7*H*-benz[*de*]anthracene-10-carboxylic acid, O-80064
7-Oxo-7*H*-benz[*de*]anthracene-11-carboxylic acid, O-80065
7-Oxo-7*H*-benz[*de*]anthracene-1-carboxylic acid, O-80058
7-Oxo-7*H*-benz[*de*]anthracene-2-carboxylic acid, O-80059
7-Oxo-7*H*-benz[*de*]anthracene-3-carboxylic acid, O-80060
7-Oxo-7*H*-benz[*de*]anthracene-4-carboxylic acid, O-80061
7-Oxo-7*H*-benz[*de*]anthracene-8-carboxylic acid, O-80062
7-Oxo-7*H*-benz[*de*]anthracene-9-carboxylic acid, O-80063

$C_{18}H_{10}O_6$
Bicoumol, B-70093
Edgeworin, E-80006

$C_{18}H_{10}O_7$
Edgeworthin, *in* D-70006

$C_{18}H_{10}O_9$
Variegatorubin, V-80003

$C_{18}H_{10}S$
Acenaphtho[1,2-*b*]benzo[*d*]thiophene, A-70016
Triphenyleno[1,12-*bcd*]thiophene, T-70310

$C_{18}H_{10}S_2$
Benzo[1,2-*b*:4,5-*b*′]bis[1]benzothiophene, B-60018
Benzo[1,2-*b*:5,4-*b*′]bis[1]benzothiophene, B-60019
Phenanthro[1,10-*bc*:8,9-*b*′,*c*′]bisthiopyran, P-60072

$C_{18}H_{11}Br$
1-Bromobenz[*a*]anthracene, B-80174
2-Bromobenz[*a*]anthracene, B-80175
3-Bromobenz[*a*]anthracene, B-80176
4-Bromobenz[*a*]anthracene, B-80177
▷ 7-Bromobenz[*a*]anthracene, B-80178
1-Bromochrysene, B-80187
2-Bromochrysene, B-80188
3-Bromochrysene, B-80189
4-Bromochrysene, B-80190
5-Bromochrysene, B-80191
6-Bromochrysene, B-80192

$C_{18}H_{11}N$
11*H*-Dibenzo[*a*,*def*]carbazole, D-80067
4*H*-Naphtho[1,2,3,4-*def*]carbazole, N-80004

$C_{18}H_{11}NO_2$
1*H*-Benz[*e*]indole-1,2(3*H*)-dione; *N*-Ph, *in* B-70026
Benz[*cd*]indol-2-(1*H*)-one; *N*-Benzoyl, *in* B-70027
7-Oxo-7*H*-benz[*de*]anthracene-11-carboxylic acid; Amide, *in* O-80065
7-Oxo-7*H*-benz[*de*]anthracene-2-carboxylic acid; Amide, *in* O-80059

$C_{18}H_{12}$
$\Delta^{1,1'}$-Biindene, B-60109
Cyclohepta[*a*]phenalene, C-60199
Cycloocta[*def*]phenanthrene, C-80187

$C_{18}H_{12}N_4$
5,14-Dihydroquinoxalino[2,3-*b*]phenazine, D-70264
[1,2,4,5]Tetrazino[1,6-*a*:4,3-*a*′]diisoquinoline, T-60172
[1,2,4,5]Tetrazino[1,6-*a*:4,3-*a*′]diquinoline, T-60173

$C_{18}H_{12}N_6$
2,4,6-Tri-2-pyridinyl-1,3,5-triazine, T-70316
2,4,6-Tri-3-pyridinyl-1,3,5-triazine, T-70317
2,4,6-Tri-4-pyridinyl-1,3,5-triazine, T-70318

$C_{18}H_{12}N_6O_6$
2*a*,4*a*,6*a*,8*a*,10*a*,12*a*-Hexaazacoronene-1,3,5,7,9,11(2*H*,4*H*,6*H*,8*H*,10*H*,12*H*)-hexone, H-80035

$C_{18}H_{12}N_{12}O_6$
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tripyrazine-2,3,6,7,10,11-tetracarboxylic acid; Hexaamide, *in* B-60051

$C_{18}H_{12}O$
Benz[*a*]anthracen-10-ol, B-80011
Benz[*a*]anthracen-11-ol, B-80012
▷ Chrysene-5,6-oxide, C-70174
3-Hydroxybenz[*a*]anthracene, H-70104
Triphenylene-1,2-oxide, T-60385

$C_{18}H_{12}O_2$
2,2′-Biindanylidene-1,1′-dione, B-80097
1,2-Di-(1-Benzofuranyl)ethylene, D-80069
1-Pyreneacetic acid, P-60208
4-Pyreneacetic acid, P-60209

$C_{18}H_{12}O_2S$
4,6-Diphenylthieno[2,3-*c*]furan, D-80514

$C_{18}H_{12}O_2S_2$
5*a*,5*b*,11*a*,11*b*-Tetrahydrocyclobuta[1,2-*b*:4,3-*b*′]benzothiopyran-11,12-dione, T-60063

$C_{18}H_{12}O_4$
9,10-Dihydro-9,10-ethenoanthracene-11,12-dicarboxylic acid, D-70208
(Diphenylpropadienylidene)propanedioic acid, D-70492
Glabone, G-60021
Kanjone, K-70003
Kanjone, K-80002
Pongone, P-70108

$C_{18}H_{12}O_4S$
5-Hydroxy-2-(phenylthio)-1,4-naphthoquinone; Ac, *in* H-70213
5-Hydroxy-3-(phenylthio)-1,4-naphthoquinone; Ac, *in* H-70214

$C_{18}H_{12}O_5$
Edulin, E-80008

$C_{18}H_{12}O_6$
Grevilline *A*, G-60038

$C_{18}H_{12}O_7$
Grevilline B, *in* G-60038
Racemic acid; Anhydride, dibenzoyl, *in* T-70005

$C_{18}H_{12}O_8$
Grevilline *D*, *in* G-60038
Grevilline C, *in* G-60038
2-Hydroxy-1,3-dimethoxy-8,9-methylenedioxycoumestan, *in* P-80029

$C_{18}H_{12}O_9$
Gomphidic acid, G-70026
Substictic acid, S-60060

$C_{18}H_{12}S$
10,11-Dihydrodiindeno[1,2-*b*:2′,1′-*d*]thiophene, D-80183

$C_{18}H_{13}N$
10,11-Dihydro-5*H*-diindeno[1,2-*b*;2′,1′-*d*]pyrrole, D-80182

$C_{18}H_{13}NO_2$
11*H*-Benzo[*a*]carbazole-1-carboxylic acid; Me ester, *in* B-80017

$C_{18}H_{13}N_3$
4-Anilino-1,10-phenanthroline, *in* A-70181
7,12-Dihydropyrido[3,2-*b*:5,4-*b*′]diindole; 7-Me, *in* D-80246
7,12-Dihydropyrido[3,2-*b*:5,4-*b*′]diindole; 12-Me; B,HCl, *in* D-80246

$C_{18}H_{13}N_3O$
Pyridazino[4,5-*b*]quinolin-10(5*H*)-one; 2-Benzyl, *in* P-80207

$C_{18}H_{14}$
1,1′-Bi-1*H*-indene, B-60108
1,1′-Bi-1*H*-indene, B-80098
2,2′-Bi-1*H*-indene, B-80099
2,3′-Bi-1*H*-indene, B-80100
3,3′-Bi-1*H*-indene, B-80101
[2.2.2](1,2,3)Cyclophane-1,9-diene, C-60229
7,12-Dihydropleiadene, D-60269
1,4-Dihydrotriphenylene, D-80262

$C_{18}H_{14}N_2$
1,2-Di-2-indolylethylene, D-80395

$C_{18}H_{14}N_2O_5$
4,4′-Diamino-2,2′-biphenyldicarboxylic acid; Anhydride, *N*,*N*′-Di-Ac, *in* D-80047

$C_{18}H_{14}N_4$
2,2′-Bis(2-imidazolyl)biphenyl, B-70148

$C_{18}H_{14}N_6$
1,4-Bis(2-pyridylamino)phthalazine, B-60172

$C_{18}H_{14}O$
2,7-Diphenyloxepin, D-60486

$C_{18}H_{14}O_2$
1,1′-Biindane-2,2′-dione, B-80095
2,2′-Biindane-1,1′-dione, B-80096
1,5-Diacetylanthracene, D-70028
1,6-Diacetylanthracene, D-70029
1,8-Diacetylanthracene, D-70030
9,10-Diacetylanthracene, D-70031
1,8-Phenanthrenedicarboxylic acid; Di-Me ester, *in* P-80078

$C_{18}H_{14}O_4$
3,4-Acenaphthenedicarboxylic acid; Di-Et ester, *in* A-60013
1,8-Anthracenedicarboxylic acid; Di-Me ester, *in* A-60281
7-Hydroxy-2-methylisoflavone; Ac, *in* H-80205
7-Hydroxy-3-methylisoflavone; Ac, *in* H-80206
Neodunol; Me ether, *in* N-80020
4-Oxo-2-phenyl-4*H*-1-benzopyran-3-carboxylic acid; Et ester, *in* O-60085
3,4-Phenanthrenedicarboxylic acid; Di-Me ester, *in* P-60068
Pongamol, P-80169

$C_{18}H_{14}O_6$
2,3-Dibenzoylbutanedioic acid, D-70083
2′,7-Dimethoxy-4′,5′-methylenedioxyisoflavone, *in* T-80107
3′,4′-Dimethoxy-6,7-methylenedioxyisoflavone, *in* T-80111
3′,4′-Dimethoxy-7,8-methylenedioxyisoflavone, *in* T-70112

4′,5-Dimethoxy-6,7-methylenedioxyisoflavone, *in* D-80341
5,7-Dimethoxy-3′,4′-methylenedioxyisoflavone, *in* T-80109
6,7-Dimethoxy-3′,4′-methylenedioxyisoflavone, *in* T-80111

$C_{18}H_{14}O_7$
3′-Hydroxy-4′,5-dimethoxy-6,7-methylenedioxyiosflavone, *in* P-80043
6-Hydroxy-2′,7-dimethoxy-4′,5′-methylenedioxyisoflavone, *in* P-80042
7-Hydroxy-2′,6-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80042
7-Hydroxy-5,6-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-70032
7-Hydroxy-5,6-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80043
7-Hydroxy-5,8-dimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80045

$C_{18}H_{14}O_8$
8-Acetoxy-2′,3,5-trihydroxy-7-methoxyflavone, *in* P-70029
2,3-Di-*O*-benzoyltartaric acid, *in* T-70005

$C_{18}H_{14}S$
Di-2-indenyl sulfide, D-80394

$C_{18}H_{15}NO_3$
10-Amino-9-anthracenecarboxylic acid; *N*-Ac, Me ester, *in* A-70088
2,2′,2″-Nitrilotrisphenol, N-70039
4,4′,4″-Nitrilotrisphenol, N-70040

$C_{18}H_{15}NO_7$
Sylvianecic acid, S-80055

$C_{18}H_{15}N_3$
Amino-1,4-benzoquinone; Dianil, *in* A-60089

$C_{18}H_{16}$
Bi(cyclononatetraenylidene), B-70104
1,1′-Biindanylidene, B-70120
1,2-Dibenzylidenecyclobutane, D-60083
1,2-Diphenyl-1,4-cyclohexadiene, D-60477
1,3,5,7-Tetraethynyladamantane, T-70025
1,2,3,4-Tetrahydrotriphenylene, T-80082
1,4,5,8-Tetrahydrotriphenylene, T-80083

$C_{18}H_{16}Cl_2O_2$
3,4-Diphenylhexanedioic acid; Dichloride, *in* D-80511

$C_{18}H_{16}N_2$
2,5-Diphenylhexanedioic acid; Dinitrile, *in* D-80510
3,4-Diphenylhexanedioic acid; Dinitrile, *in* D-80511

$C_{18}H_{16}N_2O_4$
5,5′-Diamino-2,2′-biphenyldicarboxylic acid; N,N′-Di-Ac, *in* D-80051

$C_{18}H_{16}N_2O_6$
2,2′-Diamino-4,4′-biphenyldicarboxylic acid; N,N′-Di-Ac, *in* D-80046
4,4′-Diamino-3,3′-biphenyldicarboxylic acid; N,N′-Di-Ac, *in* D-80049

$C_{18}H_{16}N_2S_2$
4,6-Diamino-1,3-benzenedithiol; Di-*S*-Ph, *in* D-70037

$C_{18}H_{16}O_2$
2,7-Dihydroxy-1,6-dimethyl-5-vinylphenanthrene, D-70294
Eupomatenoid 6, E-60075

$C_{18}H_{16}O_3$
2-(2-Hydroxy-4-methoxyphenyl)-5-(1-propenyl)benzofuran, *in* H-60214
6-Hydroxy-7,9-octadecadiene-11,13,15,17-tetraynoic acid, H-70195
2-(4-Hydroxyphenyl)-7-methoxy-5-(1-propenyl)benzofuran, *in* H-60214
2-(4-Hydroxyphenyl)-3-methyl-5-(2-oxopropyl)benzofuran, *in* H-80236

$C_{18}H_{16}O_4$
3-Butene-1,2-diol; Dibenzoyl, *in* B-70291
2-(2,4-Dihydroxyphenyl)-7-methoxy-5-(1-propenyl)benzofuran, *in* H-60214
2,2′-Dihydroxystilbene; Di-Ac, *in* D-80378
3,5-Dihydroxystilbene; Di-Ac, *in* D-80384
4,4′-Dihydroxystilbene; Di-Ac, *in* D-80385

$C_{18}H_{16}O_4Se_2$
2,3-Bis(phenylseleno)-2-butenedioic acid; Di-Me ester, *in* B-80159

$C_{18}H_{16}O_5$
4-Angeloyloxy-8,9-epoxy-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]non-2-ene, *in* M-80202
1,3-Dihydroxy-2-hydroxymethylanthraquinone; Tri-Me ether, *in* D-70306
▷ 2-Ethoxymethyl-3-hydroxy-1-methoxyanthraquinone, *in* D-70306
Globuxanthone, G-80020
5-Hydroxy-4′,7-dimethoxy-6-methylflavone, *in* T-80326
Intricatin, *in* I-80017
8-Methoxybonducellin, *in* B-60192
Puerol *B*, *in* P-70137
1,3,6-Trihydroxy-2-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, T-80325
5,6,7-Trimethoxyflavone, *in* T-60322
2′,4′,7-Trimethoxyisoflavone, *in* T-70264
3′,4′,7-Trimethoxyisoflavone, *in* T-80308
4′,6,7-Trimethoxyisoflavone, *in* T-80310
4′,7,8-Trimethoxyisoflavone, *in* T-70265
1,2,8-Trimethoxy-3-methylanthraquinone, *in* T-80322

$C_{18}H_{16}O_6$
2,3,4-Biphenyltriol; Tri-Ac, *in* B-70124
6,7-Dimethoxy-3′,4′-methylenedioxyflavanone, *in* T-70106
6,7-Dimethoxy-3′,4′-methylenedioxyisoflavanone, *in* T-80102
2,3-Dimethoxy-8,9-methylenedioxypterocarpan, *in* T-80117
3,4-Dimethoxy-8,9-methylenedioxypterocarpan, *in* T-80119
5-Hydroxy-2′,6,6′-trimethoxyflavone, *in* T-70107
2′-Hydroxy-3′,4′,7-trimethoxyisoflavone, *in* T-80105
5-Hydroxy-4′,6,7-trimethoxyisoflavone, *in* T-80112
7-Hydroxy-2′,4′,5′-trimethoxyisoflavone, *in* T-80107
7-Hydroxy-3′,4′,6-trimethoxyisoflavone, *in* T-80111
7-Hydroxy-4′,5,6-trimethoxyisoflavone, *in* T-80112
7-Hydroxy-4′,5,8-trimethoxyisoflavone, *in* T-80113
Isoamericanin *A*, I-60087
Pedicellosine, P-70015
Scleroderolide, S-60013
1,3,5,8-Tetrahydroxy-2-(3-methyl-2-butenyl)xanthone, T-60114
2′,5′,6-Trihydroxy-3,5,7-trimethoxyflavone, *in* H-60064
3′,4′,5-Trihydroxy-3,6,7-trimethoxyflavone, *in* H-80067

$C_{18}H_{16}O_7$
Arizonin C_1, A-70254
3,4′-Dihydroxy-5,6,7-trimethoxyflavone, *in* P-80035
3,5-Dihydroxy-4′,6,7-trimethoxyflavone, *in* P-80035
4′,5-Dihydroxy-3,6,7-trimethoxyflavone, *in* P-80035
4′,5-Dihydroxy-3,6,8-trimethoxyflavone, *in* P-60048
5,6-Dihydroxy-3,4′,8-trimethoxyflavone, *in* P-60048
5,7-Dihydroxy-3,4′-6-trimethoxyflavone, *in* P-80035
5,7-Dihydroxy-3,6,8-trimethoxyflavone, *in* P-70031
3′,8-Dihydroxy-4′,7,8-trimethoxyisoflavone, *in* P-80046
4′,5-Dihydroxy-2′,5′,7-trimethoxyisoflavone, *in* P-80041
5,7-Dihydroxy-3′,4′,7-trimethoxyisoflavone, *in* P-80043
5,7-Dihydroxy-3′,4′,8-trimethoxyisoflavone, *in* P-80045
6*a*-Hydroxy-2,3-dimethoxy-8,9-methylenedioxypterocarpan, *in* P-80052
Notatic acid, N-70081
Psorospermindiol; *O*-De-Me, epimer, *in* P-70133

$C_{18}H_{16}O_8$
4′,5,7-Trihydroxy-3′,6,8-trimethoxyflavone, T-80341
2′,3′,5-Trihydroxy-3,7,8-trimethoxyflavone, *in* H-70079
2′,5,5′-Trihydroxy-3,7,8-trimethoxyflavone, *in* H-70080
3′,4′,5-Trihydroxy-5′,6,7-trimethoxyflavone, *in* H-70081
3′,5,7-Trihydroxy-4′,5′,6-trimethoxyflavone, *in* H-70081
3′,5,7-Trihydroxy-4′,5′,6-trimethoxyisoflavone, *in* H-80071

$C_{18}H_{16}O_9$
Alectorialic acid, A-70081
Decarboxythamnolic acid, D-80014
3′,5,5′,7-Tetrahydroxy-3,4′,8-trimethoxyflavone, *in* H-70021

$C_{18}H_{16}O_{10}$
3′,4′,5,5′,7-Pentahydroxy-3,6,8-trimethoxyflavone, *in* O-70018

$C_{18}H_{17}ClO_7$
Wrightiin, W-80005

$C_{18}H_{17}N$
2,2-Dimethyl-4,4-diphenyl-3-butenoic acid; Nitrile, *in* D-70402

$C_{18}H_{17}NO_2$
10-Amino-9-anthracenecarboxylic acid; *N*-Di-Me, Me ester, *in* A-70088

$C_{18}H_{17}NO_5$
2-Amino-4-hydroxybutanoic acid; *O*,*N*-Dibenzoyl, *in* A-70156
2-Amino-3-phenylpentanedioic acid; *N*-Benzoyl, *in* A-60241

$C_{18}H_{18}$
2-*tert*-Butylphenanthrene, B-70305
3-*tert*-Butylphenanthrene, B-70306
9-*tert*-Butylphenanthrene, B-70307
[2.2.2](1,2,3)Cyclophane, C-60228
1,2,3,4,7,8-Hexahydrobenzo[*c*]phenanthrene, H-80052
1,2,3,6,7,8-Hexahydro-3*a*,5*a*-ethenopyrene, H-70056
1,5,9,10-Tetramethylanthracene, T-80137
1,8,9,10-Tetramethylanthracene, T-80138
1,3,6,8-Tetramethylphenanthrene, T-60151
2,4,5,7-Tetramethylphenanthrene, T-60152

$C_{18}H_{18}O$
2,2-Dimethyl-4,4-diphenyl-3-butenal, D-70401

$C_{18}H_{18}O_2$
Conocarpan, C-60161
2,2-Dimethyl-4,4-diphenyl-3-butenoic acid, D-70402
5,5-Diphenyl-4-pentenoic acid; Me ester, *in* D-80513

$C_{18}H_{18}O_3$
Dehydroallogibberic acid, *in* A-80045
2-(4-Hydroxyphenyl)-5-(2-Hydroxypropyl)-3-methylbenzofuran, H-80236
Olmecol, O-60040

$C_{18}H_{18}O_3S$
1-(2-Furyl)-4[5-(isovaleryloxymethyl)-2-thienyl]-1-buten-3-yne, *in* F-80093

$C_{18}H_{18}O_4$
Bharanginin, B-70089
Bibenzyl-2,2′-dicarboxylic acid; Di-Me ester, *in* B-80071
Ceroptene, C-80038
2,5-Diphenylhexanedioic acid, D-80510
3,4-Diphenylhexanedioic acid, D-80511
1,2,5,6-Tetramethoxyphenanthrene, *in* T-60115

1,2,5,7-Tetramethoxyphenanthrene, *in* T-80114
1,2,6,7-Tetramethoxyphenanthrene, *in* T-60117
1,3,5,6-Tetramethoxyphenanthrene, *in* T-60118
1,3,6,7-Tetramethoxyphenanthrene, *in* T-60119
2,3,5,7-Tetramethoxyphenanthrene, *in* T-60120
2,3,6,7-Tetramethoxyphenanthrene, *in* T-60121
2,4,5,6-Tetramethoxyphenanthrene, *in* T-60122
3,4,5,6-Tetramethoxyphenanthrene, *in* T-60123
2′,4′,6′-Trimethoxychalcone, *in* P-80139

$C_{18}H_{18}O_5$
5,6-Dimethoxy-3-(4-methoxybenzyl)phthalide, D-60398
Echinofuran, E-60002
Homocyclolongipesin; Ac, *in* H-60088
3-(4-Hydroxyphenyl)-1-(2-hydroxy-4,6-dimethoxyphenyl)-2-propen-1-one, *in* H-80246
2,3,9-Trimethoxypterocarpan, *in* T-80335
3,4,9-Trimethoxypterocarpan, *in* T-80336

$C_{18}H_{18}O_6$
Alkannin acetate, *in* S-70038
Curvularin; 10,11-Didehydro(*E*-), 7-Ac, *in* C-80166
5,8-Dihydroxy-6,10-dimethoxy-2-propyl-4*H*-naphtho[2,3-*b*]pyran-4-one, D-70292
5,8-Dihydroxy-2,3,6,7-tetramethyl-1,4-naphthoquinone; Di-Ac, *in* D-60377
1-(2,5-Dihydroxy-3,4,6-trimethoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80050
7-Hydroxy-2′,5,8-trimethoxyflavanone, *in* T-70104
2′-Hydroxy-3′,4′,7-trimethoxyisoflavanone, *in* T-80099
7-Hydroxy-2′,3′,4′-trimethoxyisoflavanone, *in* T-80099
Monocillin *I*, *in* N-60060
Shikonin acetate, *in* S-70038
3,4,7,8-Tetramethoxy-2,6-phenanthrenediol, *in* H-60066

$C_{18}H_{18}O_7$
2,8-Dihydroxy-3,9,10-trimethoxypterocarpan, *in* P-80054
Monomethylsulochrin, *in* S-70083
1,2,3,4,8-Pentamethoxyxanthone, *in* P-60051
Senepoxide, S-60023
β-Senepoxide, *in* S-60023
3′,4′,5,6-Tetrahydroxy-7-methoxyflavanone, *in* P-70028

$C_{18}H_{18}O_8$
Arizonin A_2, *in* A-70255
Arizonin B_2, *in* A-70255

$C_{18}H_{19}NO$
2,2-Dimethyl-4,4-diphenyl-3-butenal; Oxime, *in* D-70401
2-Phenylcyclopentylamine; Benzoyl, *in* P-60086
2-Phenylcyclopentylamine; *N*-Benzoyl, *in* P-60086

$C_{18}H_{19}NO_3S$
2-Amino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylic acid; Et ester, *N*-benzoyl, *in* A-60258

$C_{18}H_{19}NO_7S$
Fibrostatin *A*, *in* F-70008

$C_{18}H_{19}NO_8S$
Fibrostatin *C*, *in* F-70008
Fibrostatin *D*, *in* F-70008
Fibrostatin *E*, *in* F-70008

$C_{18}H_{19}N_3O_5S$
Antibiotic BMY 28100, A-70221

$C_{18}H_{20}$
3,3-Dimethyl-4,4-diphenyl-1-butene, D-60418
5,13-Dimethyl[2.2]metacyclophane, D-60426

$C_{18}H_{20}N_2O_2$
5,6-Acenaphthenedicarboxylic acid; Bis(dimethylamide), *in* A-70015
2,2′-Diamino-4,4′-biphenyldicarboxylic acid; Di-Et ester, *in* D-80046

$C_{18}H_{20}N_2O_4$
N-Tyrosylphenylalanine, T-60412

$C_{18}H_{20}N_4$
Tricyclo[3.3.1.1^{3,7}]decane-1,3,5,7-tetraacetonitrile, *in* A-70064

$C_{18}H_{20}O_2$
Pentamethylphenol; Benzoyl, *in* P-60058
Salviolone, S-70006
3,5-Tridecadiene-7,9,11-triyn-1-ol; 3-Methylbutanoyl, *in* T-80258

$C_{18}H_{20}O_3$
Allogibberic acid, A-80045
2,3-Dihydro-2-(4-hydroxyphenyl)-5-(3-hydroxypropyl)-3-methylbenzofuran, D-60244
1-(4-Hydroxyphenyl)-2-(4-propenylphenoxy)-1-propanol, H-60215
Tetrahydrobis(4-hydroxyphenyl)-3,4-dimethylfuran, T-60061

$C_{18}H_{20}O_4$
Angoletin, A-80156
2,5-Dihydroxy-3,6-dimethyl-3,6-diphenyl-1,4-dioxan, *in* H-80240
4,6,12-Tetradecatriene-8,10-diyne-1,3-diol; Di-Ac, *in* T-80033
Thujin, T-70190

$C_{18}H_{20}O_5$
9,10-Dihydro-7-hydroxy-2,3,4,6-tetramethoxyphenanthrene, *in* D-70246
Longipesin; Propanoyl, *in* L-60034
9-Methyllongipesin; O^9-Ac, *in* M-70091
Monocillin II, *in* N-60060

$C_{18}H_{20}O_6$
3,3′-Dihydroxy-4′,5,7-trimethoxyflavan, *in* P-70026
3,4′-Dihydroxy-3′,5,7-trimethoxyflavan, *in* P-70026
3′,7-Dihydroxy-2′,4′,8-trimethoxyisoflavan, *in* P-80038
Epicatechin; $O^{3'}$,O^5,O^7-Tri-Me, *in* P-70026
3-Methoxy-6-[2-(3,4-5-trimethoxyphenyl)ethenyl]-1,2-benzenediol, *in* T-60344
Monocillin III, *in* N-60060
Syringopicrogenin *A*, S-60067

$C_{18}H_{20}O_7$
Arnebin VI, *in* D-80343
Syringopicrogenin *B*, *in* S-60067
2′,6,8-Trihydroxy-3′,4′,7-trimethoxyisoflavan, *in* H-80068

$C_{18}H_{20}Se_2$
9,18-Dimethyl-2,11-diselena[3.3]metacyclophane, D-70404

$C_{18}H_{21}N_3O_6$
10-Deazariboflavin, *in* P-60245

$C_{18}H_{22}N_2O_3S_2$
Dithiosilvatin, D-60511

$C_{18}H_{22}N_4$
5,5*a*,6,11,11*a*,12-Hexahydroquinoxalino[2,3-*b*]quinoxaline; *N*-Tetra-Me, *in* H-80066

$C_{18}H_{22}O_2$
2,3-Dimethoxy-2,3-diphenylbutane, *in* D-80505
15-Octadecene-9,11,13-triynoic acid, O-80009

$C_{18}H_{22}O_3$
Nimbinone, N-70037
Nimbione, N-70038

$C_{18}H_{22}O_4$
1,12-Diacetoxy-4,6-tetradecadiene-8,10-diyne, *in* T-80026
12-Hydroxy-13-methoxy-8,11,13-podocarpatriene-3,7-dione, *in* N-80028
6,12-Tetradecadiene-8,10-diyne-1,3-diol; Di-Ac, *in* T-80027

$C_{18}H_{22}O_5$
1-(4-Hydroxy-3-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)-ethane, *in* D-80371
Monocillin IV, *in* N-60060
▷ Zearalenone, Z-60002

$C_{18}H_{22}O_6$
Combretastatin, C-70192
8′-Hydroxyzearalenone, *in* Z-60002
3-Methoxy-6-[2-(3,4,5-trimethoxyphenyl)ethyl]1,2-benzenediol, *in* T-60344
Monocillin V, *in* N-60060

$C_{18}H_{22}O_7$
1-(4-Hydroxy-3-methoxyphenyl)-2-(4-hydroxy-3,5-dimethoxyphenyl)-1,3-propanediol, *in* B-80150

$C_{18}H_{22}O_{11}$
Tectoridin, *in* T-80319

$C_{18}H_{23}NO_2$
3,7-Di-*tert*-butyl-1-nitronaphthalene, D-80110

$C_{18}H_{23}NO_3$
2,6-Di-*tert*-butyl-1-nitronaphthalene, D-80109

$C_{18}H_{24}$
1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydrotriphenylene, D-60516
1,3,5,7-Tetravinyladamantane, T-70154

$C_{18}H_{24}N_2$
1,2-Diphenyl-1,2-ethanediamine; *N*-Tetra-Me, *in* D-70480

$C_{18}H_{24}O_2$
1-Acetoxy-6,8,12,14-hexadecatetraen-10-yne, *in* H-80041
3-(2-Hydroxy-4,8-dimethyl-3,7-nonadienyl)benzaldehyde, H-60122
Nimbiol, N-80027
Norsalvioxide, N-70079

$C_{18}H_{24}O_4$
3-Acetoxy-6-methoxyprimnatrienone, *in* P-80174
Nimbionol, N-80028
2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)acetophenone, T-80289

$C_{18}H_{24}O_5$
Nordinone, N-60060

$C_{18}H_{24}O_7$
Malabarolide, M-70008
Nordinonediol, *in* N-60060

$C_{18}H_{24}O_8$
1,3,5,7-Adamantanetetraacetic acid, A-70064
1,3,5,7-Adamantanetetracarboxylic acid; Tetra-Me ester, *in* A-80037
Hyptolide, H-70236

$C_{18}H_{24}O_{12}$
myo-Inositol; Hexa-Ac, *in* I-80015

$C_{18}H_{26}O_3$
Ecklonialactone A, E-80005

$C_{18}H_{26}O_4$
3-Deoxybarbacenic acid, *in* B-80009

$C_{18}H_{26}O_5$
Barbacenic acid, B-80009

$C_{18}H_{26}O_6$
3-Oxo-17-carboxy-3,18-secobarbacenic acid, O-80071

$C_{18}H_{26}O_8$
Boronolide, B-60193

$C_{18}H_{27}N_3$
1,3,5-Tripyrrolidinobenzene, T-70319

$C_{18}H_{27}N_3O_3$
1,3,5-Trimorpholinobenzene, T-70294

$C_{18}H_{28}$
9,9′-Bi(bicyclo[3.3.1]nonylidene), B-60079

$C_{18}H_{28}BF_4NO_2$
1,1-*tert*-Butyl-3,3-diethoxy-2-azaallenium(1+); Tetrafluoroborate, *in* B-70301

$C_{18}H_{28}O_2$
11,17-Octadecadien-9-ynoic acid, O-80006
4,8,12,15-Octadecatetraenoic acid, O-80008
Spiro[3,4-cyclohexano-4-hydroxybicyclo[3.3.1]nonan-9-one-2,1′-cyclohexane], S-70063

$C_{18}H_{28}O_3$
ent-6β,17-Dihydroxy-14,15-bisnor-7,11*E*-labdadien-13-one, D-60311
14,15-Dinor-13-oxo-7-labden-17-oic acid, D-70457
Ecklonialactone B, *in* E-80005
2-Hydroxy-6-undecylbenzoic acid, H-80264

$C_{18}H_{28}O_4$
ent-12-Hydroxy-13,14,15,16-tetranor-1(10)-halimen-18-oic acid; Ac, *in* H-60231
Xestodiol, X-70006

$C_{18}H_{28}O_5$
Lachnellulone, L-70015

$C_{18}H_{28}S_6$
1,3,4,6-Tetrakis(isospropylthio)thieno[3,4-*c*]thiophene, *in* T-70170

$C_{18}H_{29}NO_2$
1,3,5-Tri-*tert*-butyl-2-nitrobenzene, T-70216

$C_{18}H_{30}$
▷ Hexaethylbenzene, H-70043
Octadecahydrotriphenylene, O-70004
1,3,5-Tributylbenzene, T-70215

$C_{18}H_{30}O_2$
5,6-Epoxy-6,10,14-trimethyl-9,13-pentadecadien-2-one, E-80047
2-Hydroxy-14,15-bisnor-7-labden-13-one, H-80133
17-Octadecen-9-ynoic acid, O-80010

$C_{18}H_{30}O_3$
Colneleic acid, C-70189
▷ Conocandin, C-70194
Sterebin *D*, S-60052

$C_{18}H_{30}O_4$
11-Hydroxy-12,13-epoxy-9,15-octadecadienoic acid, H-70127
Secoisoobtusilactone, S-80015
Sterebin *A*, *in* S-60052
3,7,11-Trimethyl-2,6,10-dodecatrienoic acid; 2,3-Dihydroxypropyl ester, *in* T-60364

$C_{18}H_{30}O_5$
Gloeosporone, G-60025

$C_{18}H_{30}O_6$
1,2:5,6-Di-*O*-cyclohexylidene-*myo*-inositol, *in* I-80015

$C_{18}H_{30}S_3$
7,14,21-Trithiatrispiro[5.1.5.1.5.1]heneicosane, *in* C-60209

$C_{18}H_{32}N_4O_8$
1,4,8,11-Tetraazacyclotetradecane-1,4,8,11-tetraacetic acid, T-60017

$C_{18}H_{32}O_2$
2,4-Octadecadienoic acid, O-70003

$C_{18}H_{32}O_3$
Feronolide, F-80004
13-Hydroxy-9,11-octadecadienoic acid, H-70196

$C_{18}H_{32}O_5$
Aspicillin, A-60312

$C_{18}H_{33}FO_2$
18-Fluoro-9-octadecenoic acid, F-80057

$C_{18}H_{34}O$
2,4-Octadecadien-1-ol, O-60004

$C_{18}H_{34}O_2$
1-Tetradecylcyclopropanecarboxylic acid, T-60040

$C_{18}H_{34}O_4$
4,14-Dihydroxyoctadecanoic acid, D-80345
11-Hydroxyhexadecanoic acid; Ac, *in* H-80172

$C_{18}H_{35}FO_2$
2-Fluorooctadecanoic acid, F-80056

$C_{18}H_{36}N_2O_6$
▷ 4,7,13,16,21,24-Hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane, H-60073

$C_{18}H_{36}N_6$
Hexakis(dimethylamino)benzene, *in* B-80014

$C_{18}H_{36}O$
2-Octadecen-1-ol, O-60007

$C_{18}H_{36}O_2$
3-Octadecene-1,2-diol, O-60005
9-Octadecene-1,12-diol, O-60006

$C_{18}H_{36}O_3$
11-Hydroxyhexadecanoic acid; Et ester, *in* H-80172
17-Hydroxyoctadecanoic acid, H-80220

$C_{18}H_{36}O_5$
9,10,18-Trihydroxyoctadecanoic acid, T-60334

$C_{18}H_{38}$
3,4-Di-*tert*-butyl-2,2,5,5-tetramethylhexane, D-70109

$C_{18}H_{38}N_2$
1,1,1′,1′-Tetra-*tert*-butylazomethane, T-60024

$C_{18}H_{38}O$
2-Octadecanol, O-80007

$C_{18}H_{39}NO_2$
Tetrabutylammonium(1+); Acetate, *in* T-80014

$C_{18}H_{39}N_3O_3$
1,9,17-Trioxa-5,13,21-triazacyclotetracosane, T-80358

$C_{18}H_{42}N_6$
1,4,7,13,16,19-Hexaazacyclotetracosane, H-70029

$C_{18}H_{42}N_6O_2$
1,13-Dioxa-4,7,10,16,20,24-hexaazacyclohexacosane, D-70459

$C_{18}N_6O_9$
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tripyrazine-2,3,6,7,10,11-tetracarboxylic acid; Trianhydride, *in* B-60051

$C_{18}N_{12}$
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tripyrazine-2,3,6,7,10,11-tetracarboxylic acid; Hexanitrile, *in* B-60051

$C_{19}Cl_{15}$
Tris(pentachlorophenyl)methyl, *in* T-60405

$C_{19}Cl_{21}Sb$
Tris(pentachlorophenyl)methyl hexachloroantimonate, *in* T-60405

$C_{19}HCl_{15}$
Tris(pentachlorophenyl)methane, T-60405

$C_{19}H_{10}O_2$
8*H*-Pyreno[2,1-*b*]pyran-8-one, P-80204
9*H*-Pyreno[1,2-*b*]pyran-9-one, P-80205

$C_{19}H_{10}O_6$
Dehydrodolineone, *in* D-80528

$C_{19}H_{11}ClO$
2-Triphenylenecarboxylic acid; Chloride, *in* T-60384

$C_{19}H_{11}N$
1-Cyanochrysene, *in* C-80128
3-Cyanochrysene, *in* C-80130
5-Cyanochrysene, *in* C-80131
6-Cyanochrysene, *in* C-80132
2-Cyanotriphenylene, *in* T-60384

$C_{19}H_{11}NO$
Dibenzo[*f*,*h*]furo[2,3-*b*]quinoline, D-80070

$C_{19}H_{11}NOS$
Dibenzo[*f*,*h*]thieno[2,3-*b*]quinoline; 1-Oxide, *in* D-70079

$C_{19}H_{11}NS$
Dibenzo[*f*,*h*]thieno[2,3-*b*]quinoline, D-70079

$C_{19}H_{12}N_2O$
Besthorn's red, B-80063

$C_{19}H_{12}N_2O_2$
Cyclohepta[1,2-*b*:1,7-*b*′]bis[1,4]benzoxazine, C-70219

$C_{19}H_{12}N_4O_7$
Benzo[*a*]quinolizinium(1+); Picrate, *in* B-70043

$C_{19}H_{12}O$
2-Triphenylenecarboxaldehyde, T-60382

$C_{19}H_{12}O_2$
2-Benzoylnaphtho[1,8-*bc*]pyran, B-70076
1-Chrysenecarboxylic acid, C-80128
2-Chrysenecarboxylic acid, C-80129
3-Chrysenecarboxylic acid, C-80130
5-Chrysenecarboxylic acid, C-80131
6-Chrysenecarboxylic acid, C-80132
1-Triphenylenecarboxylic acid, T-60383
2-Triphenylenecarboxylic acid, T-60384

$C_{19}H_{12}O_3$
7-Oxo-7*H*-benz[*de*]anthracene-10-carboxylic acid; Me ester, *in* O-80064
7-Oxo-7*H*-benz[*de*]anthracene-11-carboxylic acid; Me ester, *in* O-80065
7-Oxo-7*H*-benz[*de*]anthracene-4-carboxylic acid; Me ester, *in* O-80061
7-Oxo-7*H*-benz[*de*]anthracene-8-carboxylic acid; Me ester, *in* O-80062
7-Oxo-7*H*-benz[*de*]anthracene-9-carboxylic acid; Me ester, *in* O-80063

$C_{19}H_{12}O_5$
1,6,8-Trihydroxy-3-methylbenz[*a*]anthracene-7,12-dione, T-70270

$C_{19}H_{12}O_6$
Bhubaneswin, *in* B-70093
Dolineone, D-80528

$C_{19}H_{12}O_7$
Daphnoretin, D-70006

$C_{19}H_{13}N$
8*H*-Indolo[3,2,1-*de*]acridine, I-70014

$C_{19}H_{13}NO_2S$
10*H*-Phenothiazine-3-carboxylic acid; *N*-Ph, *in* P-70057

$C_{19}H_{13}NO_4S$
10*H*-Phenothiazine-3-carboxylic acid; *N*-Ph, 5,5-dioxide, *in* P-70057

$C_{19}H_{13}NO_8$
Protetrone, P-70124

$C_{19}H_{14}$
4*b*,10*b*-Methanochrysene, M-70040

$C_{19}H_{14}N_4$
4-Amino-1,2,3-benzotriazine; 3,*N*(4)-Di-Ph, *in* A-60092

$C_{19}H_{14}O$
3-Methoxybenz[*a*]anthracene, *in* H-70104

$C_{19}H_{14}OS$
9-(Phenylsulfinyl)-9*H*-fluorene, *in* F-80015

$C_{19}H_{14}O_2$
1-Pyreneacetic acid; Me ester, *in* P-60208
4-Pyreneacetic acid; Me ester, *in* P-60209

$C_{19}H_{14}O_2S$
9-(Phenylsulfonyl)-9*H*-fluorene, *in* F-80015

$C_{19}H_{14}O_4$
4′,7-Dimethoxyisoflavone, *in* D-80323
Ochromycinone, O-60003

$C_{19}H_{14}O_6$
4′,7-Dihydroxyisoflavone; Di-Ac, *in* D-80323
Ficinin, *in* E-80008

$C_{19}H_{14}O_7$
6-Aldehydoisoophiopogone *A*, A-60071

$C_{19}H_{14}O_8$
1,3,7-Trihydroxyxanthone; Tri-Ac, *in* T-80347

$C_{19}H_{14}O_{10}$
Constictic acid, C-60163

$C_{19}H_{14}S$
9-(Phenylthio)-9*H*-fluorene, *in* F-80015

$C_{19}H_{14}S_2$
2-Dibenzothiophenethiol; *S*-Benzyl, *in* D-60078
4-Dibenzothiophenethiol; *S*-Benzyl, *in* D-60079

$C_{19}H_{15}N_3$
Azidotriphenylmethane, A-60352

$C_{19}H_{16}$
4-(2,4,6-Cycloheptatrien-1-ylidene)bicyclo[5.4.1]dodeca-2,5,7,9,11-pentaene, C-60207

$C_{19}H_{16}O$
2,5-Dimethyl-3,4-diphenyl-2,4-cyclopentadien-1-one, D-70403

$C_{19}H_{16}O_4$
1,7-Bis(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, *in* C-80165
4-Cyclopentene-1,3-diol; Dibenzoyl, *in* C-80193
2-(4-Hydroxyphenyl)-7-methoxy-5-(1-propenyl)-3-benzofurancarboxaldehyde, H-60212
Moracin *D*, M-60143
Moracin *E*, M-60144
Moracin *G*, M-60145

$C_{19}H_{16}O_5$
Ambonane, *in* N-80020
3′,4′-Deoxypsorospermin, D-60021
Neoraunone, *in* N-80025

$C_{19}H_{16}O_6$
6-Aldehydoisoophiopogone *B*, A-60072
4′,7-Dihydroxyisoflavanone; Di-Ac, *in* D-80322
Psorospermin, P-70132

$C_{19}H_{16}O_7$
Fridamycin *E*, *in* F-70043
5′-Hydroxypsorospermin, *in* P-70132
2′,6,7-Trimethoxy-4′,5′-methylenedioxyisoflavone, *in* P-80042
3′,4′,8-Trimethoxy-6,7-methylenedioxyisoflavone, *in* P-80046
3′,6,7-Trimethoxy-4′,5′-methylenedioxyisoflavone, *in* P-80044
5,6,7-Trimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-70032
5,6,7-Trimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80043
6,7,8-Trimethoxy-3′,4′-methylenedioxyisoflavone, *in* P-80046

$C_{19}H_{16}O_{13}$
Heaxahydroxydiphenic acid α-L-arabinosediyl ester, H-80003

$C_{19}H_{17}ClO_6$
3′,4′-Deoxy-4′-chloropsorospermin-3′-ol, *in* D-60021

$C_{19}H_{17}N$
3,5-Dimethyl-2,6-diphenylpyridine, D-80447

$C_{19}H_{17}NO_2$
2-Hydroxycyclononanone; Oxime, *in* H-60112

$C_{19}H_{18}$
Bicyclo[12.4.1]nonadeca-1,3,5,7,9,11,13,15,17-nonaene, B-80081
Bicyclo[12.4.1]nonadec-1,3,5,7,9,11,13,15,17-nonaene, B-70101

$C_{19}H_{18}N_2$
3,3′-Methylenebisindole; 1,1′-Di-Me, *in* M-80078
(Triphenylmethyl)hydrazine, T-60388

$C_{19}H_{18}O_3$
Eupomatenoid 5, *in* E-60075
1-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]-2-(3,5-dihydroxyphenyl)ethylene, H-70167
Kachirachirol *A*, *in* K-60001
Ratanhiaphenol III, R-80003

$C_{19}H_{18}O_4$
1,2-Cyclopentanediol; Dibenzoyl, *in* C-80189
Demethylfruticulin *A*, *in* F-60076
1,2-Diphenyl-1,2-cyclopropanedicarboxylic acid; Di-Me ester, *in* D-80509
2-(2-Hydroxy-4-methoxyphenyl)-7-methoxy-5-(1-propenyl)benzofuran, *in* H-60214
Isotanshinone IIB, I-60138
6-Methoxy-2-[2-(4-methoxyphenyl)ethyl]-4*H*-1-benzopyran-4-one, M-60039
Moracin *C*, *in* M-60146

$C_{19}H_{18}O_5$
Benzophenone-2,2′-dicarboxylic acid; Di-Et ester, *in* B-70041
7-[[4-(2,5-Dihydro-4-methyl-5-oxo-2-furanyl)-3-methyl-2-butenyl]oxy]-2*H*-1-benzopyran-2-one, D-80223
1,6-Dihydroxy-3-methoxy-2-(3-methyl-2-butenyl)xanthone, *in* T-80325
Egonol, E-70001

$C_{19}H_{18}O_6$
Ciliarin, *in* C-70007
Cudraniaxanthone, C-80163
7-[[3-[(2,5-Dihydro-4-methyl-5-oxo-2-furanyl)methyl]-3-methyloxiranyl]methoxy]-2*H*-1-benzopyran-2-one, *in* D-80223
Fruticulin B, F-60077
Munduserone, M-80196
2′,5,6,6′-Tetramethoxyflavone, *in* T-70107
3′,4′,5,6-Tetramethoxyflavone, *in* T-70108
3′,4′,6,7-Tetramethoxyflavone, *in* T-80092
2′,4′,5′,7-Tetramethoxyisoflavone, *in* T-80107
3′,4′,5′,7-Tetramethoxyisoflavone, *in* T-80110
3′,4′,6,7-Tetramethoxyisoflavone, *in* T-80111
1,5,8-Trihydroxy-3-methyl-2-(3-methyl-2-butenyl)xanthone, *in* T-60114

$C_{19}H_{18}O_7$
3′,4′-Deoxypsorospermin-3′,4′-diol, *in* D-60021
Gerontoxanthone D, G-80015
5-Hydroxy-2′,3,7,8-tetramethoxyflavone, *in* P-70029
5-Hydroxy-2′,4′,7,8-tetramethoxyflavone, *in* P-80034
5-Hydroxy-3,4′,6,7-tetramethoxyflavone, *in* P-80035
5-Hydroxy-2′,4′,5′,7-tetramethoxyisoflavone, *in* P-80041
7-Hydroxy-2′,4′,5′,6-tetramethoxyisoflavone, *in* P-80042
Psorospermindiol, P-70133
Sermundone, *in* M-80196

$C_{19}H_{18}O_8$
2′-Acetoxy-3,5-dihydroxy-7,8-dimethoxyflavone, *in* P-60045
3′,5-Dihydroxy-4′,6,7,8-tetramethoxyflavone, D-60375
5,7-Dihydroxy-3′,4′,6,8-tetramethoxyflavone, D-60376
4′,5-Dihydroxy-3,3′,6,7-tetramethoxyflavone, *in* H-80067
4′,5-Dihydroxy-3,3′,6,7-tetramethoxyflavone, *in* H-80067
4′,5-Dihydroxy-3′,5′,6,7-tetramethoxyflavone, *in* H-70081
5′,5′-Dihydroxy-2′,3,7,8-tetramethoxyflavone, *in* H-70080
5,7-Dihydroxy-3′,4′,5′,6-tetramethoxyflavone, *in* H-70081
5,7-Dihydroxy-2′,4′,5′,6-tetramethoxyisoflavone, *in* H-80069
5,7-Dihydroxy-2′,4′,5′,8-tetramethoxyisoflavone, *in* H-80070
5,7-Dihydroxy-3′,4′,5′,6-tetramethoxyisoflavone, *in* H-80071
5′,6-Dihydroxy-2′,3,5,7-trimethoxyflavone, *in* H-60064

$C_{19}H_{18}O_9$
3,4′,5-Trihydroxy-3′,6,7,8-tetramethoxyflavone, *in* H-80028
3′,5,5′-Trihydroxy-3,4′,7,8-tetramethoxyflavone, *in* H-70021
3′,5,5′-Trihydroxy-4′,6,7,8-tetramethoxyflavone, *in* H-80029
3′,5,7-Trihydroxy-3,4′,5′,8-tetramethoxyflavone, *in* H-70021
3′,5,7-Trihydroxy-4′,5′,6,8-tetramethoxyflavone, *in* H-80029

$C_{19}H_{18}O_{10}$
2′,4′,5,7-Tetrahydroxy-3,5′,6,8-tetramethoxyflavone, *in* O-60022
2′,5,5′,7-Tetrahydroxy-3,4′,6,8-tetramethoxyflavone, *in* O-60022
3′,5,5′,6-Tetrahydroxy-3,4′,7,8-tetramethoxyflavone, *in* O-70018
3′,5,5′,7-Tetrahydroxy-3,4′,6,8-tetramethoxyflavone, *in* O-70018
2′,5,7-Trihydroxy-3,4′,5′,6,8-pentamethoxyflavone, *in* O-60022

$C_{19}H_{18}O_{11}$
1,3,5,8-Tetrahydroxyxanthone; 8-Glucoside, *in* T-70123

$C_{19}H_{19}ClO_7$
Eriodermic acid, E-70032
Methyl 5-chloro-4-*O*-*demethylbarbatate*, *in* B-70007

$C_{19}H_{20}$
1-Methyl-4,4-diphenylcyclohexene, M-60065
3-Methyl-4,4-diphenylcyclohexene, M-60066

$C_{19}H_{20}O_2$
3,3-Dimethyl-5,5-diphenyl-4-pentenoic acid, D-60420
Hermosillol, H-60029

$C_{19}H_{20}O_3$
Cryptotanshinone, C-60173
2,3-Dihydro-2-(4-hydroxy-3-methoxyphenyl)-3-methyl-5-(1-propenyl)benzofuran, *in* C-60161
2,3-Dihydro-2-(4-hydroxyphenyl)-7-methoxy-3-methyl-5-(1-propenyl)benzofuran, *in* C-60161
2,2′-Dihydroxy-3-methoxy-5,5′-di-2-propenylbiphenyl, D-80334
Zapotecone, *in* Z-80001

$C_{19}H_{20}O_4$
Galipein, G-60001
Honyudisin, H-70093
Kachirachirol *B*, K-60001
Nordentatin, N-80079
Umbelliferone 8-oxogeranyl ether, U-80001

$C_{19}H_{20}O_5$
Homocyclolongipesin; Propanoyl, *in* H-60088
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one; Tetra-Me ether, *in* H-80246
2,3,4,7,9-Pentamethoxyphenanthrene, *in* P-70035
Teuchamaedryn *A*, T-70157

$C_{19}H_{20}O_6$
Asadanin, A-60308
Calaxin, C-70007
Isoteucrin H_4, I-80093
Khellactone; O^{10}-Angeloyl, *in* K-70013
Khellactone; O^9-Angeloyl, *in* K-70013
1(10)*E*,8E-Millerdienolide, *in* M-60136
2′,4′,5,7-Tetramethoxyisoflavanone, *in* T-80100

$C_{19}H_{20}O_7$
Annulin *A*, A-60276
Barbatic acid, B-70007
4β,15-Epoxy-1(10)*E*,8E-millerdienolide, *in* M-60136
8-Hydroxy-3,4,9,10-tetramethoxypterocarpan, *in* P-80055
Isoelephantopin, I-60099

$C_{19}H_{20}O_8$
2,8-Dihydroxy-3,4,9,10-tetramethoxypterocarpan, *in* H-80072
Eximin, *in* A-70248

$C_{19}H_{21}NO_8S$
Fibrostatin *B*, *in* F-70008

$C_{19}H_{21}NO_9S$
Fibrostatin *F*, *in* F-70008

$C_{19}H_{22}N_2O_2$
2,4-Pentanediamine; N^2,N^4-Dibenzoyl, *in* P-70039

$C_{19}H_{22}O_2$
5-Hydroxy-1,7-diphenyl-3-heptanone, *in* D-70481

$C_{19}H_{22}O_3$
Auraptene/, A-80187
Gravelliferone, G-60037
1-(4-Hydroxyphenyl)-2-(2-methoxy-5-propenylphenyl)-2-propanol, H-80237
Miltiodiol, M-70149
Zapotecol, Z-80001

$C_{19}H_{22}O_4$
Chalepin, C-60031
t-Dehydrocrotonin, *in* C-80158
2,3-Dihydro-2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-3-methylbenzofuran, *in* D-60244
1,5-Dihydroxy-1,7-diphenyl-3-heptanone, *in* D-60480
6′,7′-Epoxyaurapten, *in* A-80187
3′,6′-Epoxycycloauraptene, E-80020
Gibberellin A_{73}, *in* G-60018
1-(4-Hydroxyphenyl)-2-(2-methoxy-4-propenylphenoxy)-1-propanol, *in* H-60215
8-Isovaleryloxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene, *in* H-70042
Neocryptotanshinone, N-60017
Tetrahydrobis(4-hydroxyphenyl)-3,4-dimethylfuran; 3′-Methoxy, *in* T-60061
Tetrahydro-2-(4-hydroxyphenyl)-5-(4-hydroxy-3-methoxyphenyl)-3,4-dimethylfuran, *in* T-60061
Yashabushiketodiol *B*, *in* D-60480

$C_{19}H_{22}O_5$
Anisocoumarin C, A-80160
ent-1α,10β-Dihydroxy-9α,15α-cyclo-20-nor-16-gibberellene-7,19-dioic acid 10,19-lactone, D-80310
Fragransol *B*, F-70042
9-Methyllongipesin; 9-Propanoyl, *in* M-70091
Subexpinnatin, *in* H-70138

$C_{19}H_{22}O_6$
Antheridic acid, A-60278
Asadanol, *in* A-60308
5-Formylzearalenone, *in* Z-60002
Isotaxiresinol, I-60139
1(10)-Millerenolide, M-60136
9-Millerenolide, M-60137
Strigol, S-60057

$C_{19}H_{22}O_7$
2′,6-Dihydroxy-3′,4′,7,8-tetramethoxyisoflavan, *in* H-80068
4β,15-Epoxy-9*E*-*millerenolide*, *in* M-60137
4β,15-Epoxy-9*Z*-*millerenolide*, *in* M-60137
Samaderine B, *in* S-80007
Tomenphantopin *B*, T-60222
Zinaflorin IV; O^6-Deacyl, O^6-(2-methylpropenoyl), *in* Z-80002

$C_{19}H_{22}O_8$
Jasmolactone A, J-80006
Syringopicrogenin *C*, *in* S-60067

$C_{19}H_{22}O_9$
Jasmolactone B, *in* J-80006

$C_{19}H_{22}O_{10}$
Aranochromanophthalide, A-60293

$C_{19}H_{23}ClO_7$
Chlororepdiolide, C-60133
Repensolide, R-60005

$C_{19}H_{23}NO$
1,2,3,4,5,6,7,8,8*a*,9*a*-Decahydrocarbazole; *N*-Benzoyl, *in* D-70012

$C_{19}H_{24}O_2$
Acalycixeniolide C, A-80012
Dehydrofalcarinol; Ac, *in* H-80021
1,7-Diphenyl-3,5-heptanediol, D-70481
1,9,15-Heptadecatriene-11,13-diyn-8-ol; Ac, *in* H-80020

$C_{19}H_{24}O_3$
1,7-Diphenyl-1,3,5-heptanetriol, D-60480

$C_{19}H_{24}O_4$
Crotonin, C-80158
t-Crotonin, *in* C-80158
12,13-Dimethoxy-8,11,13-podocarpatriene-3,7-dione, *in* D-80374
Gibberellin A_9, G-60018

$C_{19}H_{24}O_5$
Cumambranolide; 8α-(2-Methylpropenoyloxy), *in* C-80164
5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-4-one, D-80342
Gibberellin A_{20}, G-70011
Gibberellin A_{40}, *in* G-60018
Gibberellin A_{45}, *in* G-60018
Gibberellin A_{51}, *in* G-60018

$C_{19}H_{24}O_6$
3β-Acetoxyhaageanolide acetate, *in* H-60001
2α-Acetoxylaurenobiolide, *in* H-70134
Afraglaucolide, A-70070
Anisocoumarin D, A-80161
Artemisiaglaucolide, *in* D-70303
Caleine *E*, C-60005
Dehydromelitensin 4-hydroxymethacrylate, *in* M-80013
Desacetylacanthospermal *A*, *in* A-60012
1α,2α-Diacetoxyalantolactone, *in* I-80046
9β,15-Diacetoxy-1(10),4,11(13)-germacratrien-12,6α-olide, *in* D-60324
Gibberellin A_{29}, *in* G-70011
Gibberellin A_{55}, *in* G-60018
Gibberellin A_{63}, *in* G-60018
Gibberellin A_{67}, *in* G-70011
Gochnatolide, G-70024
Isoafraglaucolide, I-70060
Ivangustin; 8-Epimer, 6α-acetoxy, Ac, *in* I-70109
Praealtin D, P-80173

$C_{19}H_{24}O_7$
Achillolide *B*, A-60061
Cedronin, C-70027
Cedronin, *in* S-80007
Cratystyolide; 1,9-Di-Ac, *in* T-70257
7-Epicedronin, *in* C-70027
Eudesmaafraglaucolide, *in* T-70258
Gibberellin A_{72}, *in* G-70011
1α-Hydroxyafraglaucolide, *in* A-70070
1β-Hydroxyafraglaucolide, *in* A-70070
1α-Hydroxyisoafraglaucolide, *in* I-70060
Ligulatin *A*, *in* D-70025
8β-(2-Methylacryloxyloxy)hirsutinolide, *in* H-80089
Samaderine C, S-80007

$C_{19}H_{24}O_8$
8β-(2-Methyl-2,3-epoxypropionyloxy)hirsutinolide, *in* H-80089
Trichogoniolide, *in* D-80007

$C_{19}H_{24}O_9$
8β-Acetoxy-10β-hydroxyhirsutinolide 13-*O*-acetate, *in* H-80089

$C_{19}H_{26}O_2$
Acalycisceniolide B′, *in* A-60011
Acalycixeniolide B, A-60011
Methylnimbiol, *in* N-80027
20-Nor-8,15-isopimaradiene-7,11-dione, *in* H-80217

$C_{19}H_{26}O_3$
2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone, D-80458
ent-1β-Hydroxy-3-nor-15-beyerene-2,12-dione, H-80216

$C_{19}H_{26}O_4$
2,4-Dihydroxy-6-methoxy-3,5-bis(3-methyl-2-butenyl)acetophenone, *in* T-80289
Subcordatolide *E*, S-70079

$C_{19}H_{26}O_5$
Cumambranolide; 8α-(2-Methylpropanoyloxy), *in* C-80164
12,13-Diacetoxy-1(10)-aromadendren-2-one, *in* D-70283
Salvicanaric acid, S-70004
Subcordatolide *D*, S-70078

$C_{19}H_{26}O_6$
Deacetylviguiestin, *in* T-70003
Gibberellin A_2, G-60017
2α-Hydroxysalvicanaric acid, *in* S-70004
Ligulatin *C*, *in* D-70025
Pulchellin diacetate, *in* P-80189
Sintenin, S-70047
Tagitinin *E*, T-70003
Zexbrevin *C*, Z-70005

$C_{19}H_{26}O_7$
14-Acetoxytetraneurin *D*, *in* T-60158
Cedronolin, *in* S-80007
1β,6α-Diacetoxy-4α-hydroxy-11-eudesmen-12,8α-olide, *in* T-70259
Resinoside, R-60006
Tetraneurin *C*, *in* T-60158

$C_{19}H_{26}O_{10}$
Ptelatoside *A*, *in* H-70209

$C_{19}H_{27}BrO_6$
Graciosallene, G-80034

$C_{19}H_{28}O_2$
Acalycixeniolide *A*, A-60010
11-Hydroxy-20-nor-8,15-isopimaradien-7-one, H-80217
Xestenone, X-70005

$C_{19}H_{28}O_4$
Coralloidin *D*, *in* E-60063
Flexilin, F-70012

$C_{19}H_{28}O_5$
3β-Acetoxy-10α-ethoxy-4,11(13)-cadinadien-12-oic acid, *in* Z-70001
1β,10α; 4α,5β-Diepoxy-8α-isobutoxyglechomanolide, *in* G-60022
1β,10α; 4α,5β-Diepoxy-8β-isobutoxyglechomanolide, *in* G-60022

$C_{19}H_{28}O_6$
Desacetyltetraneurin *D* 15-*O*-isobutyrate, *in* T-60158
Desacetyltetraneurin *D* 4-*O*-isobutyrate, *in* T-60158

$C_{19}H_{28}O_7$
Tagitinin *A*, T-60002

$C_{19}H_{28}O_{11}$
7-Acetylsecologanol, *in* S-80016

$C_{19}H_{28}O_{12}$
6-*O*-Acetylshanghiside methyl ester, *in* S-60028
Barlerin, *in* S-60028

$C_{19}H_{30}N_6O_8$
Antiarrhythmic peptide (ox atrium), A-60283

$C_{19}H_{30}O_2$
Glaciolide, G-80018
Gracilin *F*, G-60035
11,17-Octadecadien-9-ynoic acid; Me ester, *in* O-80006

$C_{19}H_{30}O_3$
3-Hydroxy-16-nor-7-pimaren-15-oic acid, H-80219
Norjuslimdiolone, N-60061
17-Nor-7-oxo-8-labden-15-oic acid, *in* H-60198

$C_{19}H_{30}O_4$
ent-6α,15,16-Trihydroxy-19-nor-4-rosen-3-one, *in* N-60061

$C_{19}H_{30}O_5$
Caucalol; Di-Ac, *in* C-80029
Shiromodiol; Di-Ac, *in* S-70039

$C_{19}H_{30}O_6$
3-Hydroxymethyl-7,11-dimethyl-2,6,11-dodecatriene-1,5,10-triol; 1,1′-Di-Ac, *in* H-70174

$C_{19}H_{30}O_8$
Icariside B_1, *in* G-70028

$C_{19}H_{32}O_2$
15-Hydroxy-17-nor-8-labden-7-one, H-60198

$C_{19}H_{32}O_3$
4,6-Dihydroxy-20-nor-2,7-cembradien-12-one, D-70323
Juvenile hormone O, J-80018

$C_{19}H_{32}O_4$
4,6-Dihydroxy-7,8-epoxy-20-nor-2-cembren-12-one, *in* D-70323

$C_{19}H_{32}O_5$
Methyl 8α-acetoxy-3α-hydroxy-13,14,15,16-tetranorlabdan-12-oate, *in* D-80387

$C_{19}H_{33}NO_2$
▷ Dysidazirine, D-80538

$C_{19}H_{34}O_2$
2,4-Octadecadienoic acid; Me ester, *in* O-70003

$C_{19}H_{34}O_3$
(−)-Coriolic acid; Me ester, *in* H-70196
2-(5-Methoxy-5-methyltetrahydro-2-furanyl)-6,10-dimethyl-5,9-undecadien-2-ol, M-80047

$C_{19}H_{34}O_5$
3,6-Epidioxy-6-methoxy-4-octadecenoic acid, E-60008

$C_{19}H_{36}N_2O_5$
▷ Lipoxamycin, L-70033

$C_{19}H_{36}O_2$
2-(2,4-Hexadiynylidene)-3,4-epoxy-1,6-dioxaspiro[4.5]decane, *in* H-70042

$C_{19}H_{37}FO_2$
2-Fluorooctadecanoic acid; Me ester, *in* F-80056

$C_{19}H_{37}NO_2$
14-Azaprostanoic acid, A-60332

$C_{19}H_{38}O_3$
17-Hydroxyoctadecanoic acid; Me ester, *in* H-80220

$C_{19}H_{38}O_5$
Phloinolic acid; Me ester, *in* T-60334

$C_{19}H_{42}N_2O_8S_2$
▷ Trimethidinium methosulphate, *in* T-70277

$C_{20}H_4Cl_4I_4O_5$
Rose bengal, R-80010

$C_{20}H_8O_4S_2$
Dibenzo[*b,i*]thianthrene-5,7,12,14-tetrone, D-70078

$C_{20}H_{10}O_2$
Indeno[1,2-*b*]fluorene-6,12-dione, I-70011

$C_{20}H_{10}O_4$
4,4′-Bi(1,2-naphthaquinone), B-80103
2,2′-Bi(1,4-naphthoquinone), B-80104
6,7-Dihydroxy-1,12-perylenedione, D-80354

$C_{20}H_{11}F$
10-Fluorobenzo[*a*]pyrene, F-80027
6-Fluorobenzo[*a*]pyrene, F-80023
7-Fluorobenzo[*a*]pyrene, F-80024
8-Fluorobenzo[*a*]pyrene, F-80025
9-Fluorobenzo[*a*]pyrene, F-80026

$C_{20}H_{11}I$
6-Iodobenzo[*a*]pyrene, I-80018

$C_{20}H_{11}N$
1*H*-Phenanthro[1,10,9,8-*cdefg*]carbazole, P-80084

$C_{20}H_{12}$
Benz[*a*]aceanthrylene, B-70009
Benz[*d*]aceanthrylene, B-60009
Benz[*k*]aceanthrylene, B-60010
▷ Benz[*e*]acephenanthrylene, B-70010
Benz[*j*]acephenanthrylene, B-70011
Cyclopenta[*cd*]pleiadene, C-80191

$C_{20}H_{12}Br_2$
2,2′-Dibromo-1,1′-binaphthyl, D-60089
4,4′-Dibromo-1,1′-binaphthyl, D-60090

$C_{20}H_{12}ClN$
6-Chlorodibenzo[*c,g*]carbazole, C-80047

$C_{20}H_{12}I_2$
2,2′-Diiodo-1,1′-binaphthyl, D-60385
4,4′-Diiodo-1,1′-binaphthyl, D-60386

$C_{20}H_{12}N_2$
Benzo[1,2-*f*:4,5-*f*′]diquinoline, B-70030

$C_{20}H_{12}N_2O_2$
Isoquinacridone, I-80086
Quinacridone, Q-80001

$C_{20}H_{12}N_4$
Cycloocta[2,1-*b*:3,4-*b*′]di[1,8]naphthyridine, C-70231
Quinolino[1″,2″:1′,2′]imidazo[4′,5′:4,5]imidazo[1,2-*a*]quinoline, Q-80003

$C_{20}H_{12}O_4$
Tetraoxaporphycene, T-70146

$C_{20}H_{12}O_5$
Halenaquinone, *in* H-60002

$C_{20}H_{12}O_6$
Altertoxin III, A-60082

$C_{20}H_{12}O_7$
Dehydropachyrrhizone, *in* P-80004

$C_{20}H_{12}S$
Anthra[1,2-*b*]benzo[*d*]thiophene, A-70214
Anthra[2,1-*b*]benzo[*d*]thiophene, A-70215
Anthra[2,3-*b*]benzo[*d*]thiophene, A-70216
Benzo[3,4]phenanthro[1,2-*b*]thiophene, B-60039
Benzo[3,4]phenanthro[2,1-*b*]thiophene, B-60040
Benzo[*b*]phenanthro[1,2-*d*]thiophene, B-70039
Benzo[*b*]phenanthro[4,3-*d*]thiophene, B-70040
Dinaphtho[1,2-*b*:1′,2′-*d*]thiophene, D-80480
Dinaphtho[1,2-*b*:2′,1′-*d*]thiophene, D-80481
Dinaphtho[1,2-*b*:2′,3′-*d*]thiophene, D-80482
Dinaphtho[2,1-*b*:1′,2′-*d*]thiophene, D-80483
Dinaphtho[2,1-*b*:2′,3′-*d*]thiophene, D-80484
Dinaphtho[2,3-*b*:2′,3′-*d*]thiophene, D-80485

$C_{20}H_{12}S_5$
2,2′:5′,2″:5″,2‴:5‴,2⁗-Quinquethiophene, Q-70010

$C_{20}H_{13}NO_2$
9-Acridinecarboxylic acid; Ph ester, *in* A-70061

$C_{20}H_{14}$
1,2-Benzo[2.2]metaparacyclophan-9-ene, B-70036
Benzo[2.2]paracyclophan-9-ene, B-80033
Dibenzo[*fg,mn*]octalene, D-80072
9,10-Dihydrodicyclopenta[*c*,g]phenanthrene, D-60219
1-(Diphenylmethylene)-1*H*-cyclopropabenzene, D-70484
[2](2,6)-Naphthaleno[2]paracyclophane-1,11-diene, N-70006

$C_{20}H_{14}N_2$
Acridin-9-ylmethylidenebenzenamine, *in* A-70060

$C_{20}H_{14}O$
1-Acetyltriphenylene, A-60059
2-Acetyltriphenylene, A-60060
10-Phenylanthrone, P-80089

$C_{20}H_{14}O_2$
Benz[*a*]anthracen-11-ol; O-Ac, *in* B-80012
1-Chrysenecarboxylic acid; Me ester, *in* C-80128
2-Chrysenecarboxylic acid; Me ester, *in* C-80129
3-Chrysenecarboxylic acid; Me ester, *in* C-80130
5-Chrysenecarboxylic acid; Me ester, *in* C-80131
6-Chrysenecarboxylic acid; Me ester, *in* C-80132
3-Hydroxybenz[*a*]anthracene; Ac, *in* H-70104
1-Triphenylenecarboxylic acid; Me ester, *in* T-60383
2-Triphenylenecarboxylic acid; Me ester, *in* T-60384

$C_{20}H_{14}O_3$
7-Oxo-7*H*-benz[*de*]anthracene-10-carboxylic acid; Et ester, *in* O-80064
7-Oxo-7*H*-benz[*de*]anthracene-2-carboxylic acid; Et ester, *in* O-80059
7-Oxo-7*H*-benz[*de*]anthracene-4-carboxylic acid; Et ester, *in* O-80061
7-Oxo-7*H*-benz[*de*]anthracene-9-carboxylic acid; Et ester, *in* O-80063
7,8,8*a*,9*a*-Tetrahydrobenzo[10,11]chryseno[3,4-*b*]oxirene-7,8-diol, T-70041

$C_{20}H_{14}O_4$
4,4′,5,5′-Tetrahydroxy-1,1′-binaphthyl, T-70102
4,4′,5,5′-Tetrahydroxy-1,1′-binaphthyl, T-80086

$C_{20}H_{14}O_5$
Halenaquinol, H-60002
Sophoracoumestan A, S-80038

$C_{20}H_{14}O_6$
Alterperylenol, A-60078
▷ Altertoxin II, A-80055
7,7′-Dimethoxy-[6,8′-bi-2*H*-benzopyran]-2,2′-dione, *in* B-70093
Jayantinin, J-80008

$C_{20}H_{14}O_7$
Alterlosin I, A-80051
Neofolin, *in* P-80003
Oreojasmin, O-70044
Pachyrrhizone, P-80004

$C_{20}H_{14}O_8S$
Halenaquinol; O^{16}-Sulfate, *in* H-60002

$C_{20}H_{14}S$
1,3-Diphenylbenzo[*c*]thiophene, D-70474
9-(Phenylthio)phenanthrene, *in* P-70049

$C_{20}H_{14}Se$
9-(Phenylseleno)phenanthrene, P-60133

$C_{20}H_{15}Br$
Bromotriphenylethylene, B-70276

$C_{20}H_{15}N$
10,11-Dihydro-5-phenyl-5*H*-dibenz[*b,f*]azepine, *in* D-70185
2,3-Diphenylindole, D-70483
5*H*,9*H*-Quino[3,2,1-*de*]acridine, Q-70006

$C_{20}H_{15}NO$
2-Acetyltriphenylene; Oxime, *in* A-60060
Isocyanatotriphenylmethane, I-80056

$C_{20}H_{15}NO_3S$
10*H*-Phenothiazine-3-carboxylic acid; *N*-Ph, Me ester, *in* P-70057

$C_{20}H_{15}NO_4S$
10*H*-Phenothiazine-3-carboxylic acid; *N*-Ph, 5,5-dioxide, Me ester, *in* P-70057

$C_{20}H_{15}N_3O_8$
Dihydroxanthommatin, D-80264

$C_{20}H_{16}$
1,2-Benzo[2.2]paracyclophane, B-70038
▷ 7,12-Dimethylbenz[*a*]anthracene, D-60405

$C_{20}H_{16}N_2$
9,10-Dihydro-9,10-ethenoanthracene-11,12-dicarboxylic acid; Di-Me ester, *in* D-70208
2,2′-Dimethyl-4,4′-biquinoline, D-60413

$C_{20}H_{16}N_2O_2$
2,5-Dihydro-3,6-diphenylpyrrolo[3,4-*c*]pyrrole-1,4-dione; 2,5-Di-Me, *in* D-70204

$C_{20}H_{16}N_2O_3$
1-[4-[6-(Diethylamino)-2-benzofuranyl]phenyl]-1*H*-pyrrole-2,5-dione, D-60170

$C_{20}H_{16}N_4O_2$
Pyrazole blue, P-70153

$C_{20}H_{16}O$
Triphenylacetaldehyde, T-80359

$C_{20}H_{16}O_3$
3-(Benzyloxy)phenol; Benzoyl, *in* B-60073

$C_{20}H_{16}O_4$
Ochromycinone methyl ether, *in* O-60003
Tetraoxaporphyrinogen, T-70147

$C_{20}H_{16}O_5$
Alpinumisoflavone, A-80050
Atalantoflavone, A-80183
2,5-Bis(hydroxymethyl)furan; Dibenzoyl, *in* B-60160
Citrusinol, C-60152
Clandestacarpin, C-80138
Derrone, D-80031
Isoderrone, I-80060
Isopsoralidin, *in* C-80152
Psoralidin, P-80186
Sojagol, S-80037

$C_{20}H_{16}O_6$
Crotarin, C-60172
Dihydroalterperylenol, *in* A-60078
7,6-(2,2-Dimethylpyrano)-3,4′,5-trihydroxyflavone, D-60449
Parvisoflavone A, P-80014
Parvisoflavone B, P-80015
Psoralidin oxide, *in* P-80186

$C_{20}H_{16}O_7$
Alterlosin II, A-80052
Corylidin, C-80152

$C_{20}H_{16}O_8$
Hydroxyversicolorone, H-70230

$C_{20}H_{16}O_{12}$
2,3,5,6,8-Pentahydroxy-1,4-naphthoquinone; Penta-Ac, *in* P-70033

$C_{20}H_{17}NO$
Triphenylacetaldehyde; Oxime, *in* T-80359

$C_{20}H_{17}N_4$
2,4,6-Triphenyl-3,4-dihydro-1,2,4,5-tetrazin-1(2*H*)-yl, T-80361

$C_{20}H_{18}$
5,6-Didehydro-1,4,7,10-tetramethyldibenzo[*ae*]cyclooctene, D-60169

$C_{20}H_{18}N_2$
1,2-Di-2-indolylethylene; *N,N′*-Di-Me, *in* D-80395

$C_{20}H_{18}N_2O$
3-Amino-1,2,3,4-tetrahydrocarbazole; N^3-Benzoyl, *in* A-60259

$C_{20}H_{18}N_4O_8$
α,α′,2-Triamino-γ,γ′,3-trioxo-3*H*-phenoxazine-1,9-dibutanoic acid, T-80209

$C_{20}H_{18}O_2$
1,1,2-Triphenyl-1,2-ethanediol, T-70311

$C_{20}H_{18}O_3$
Isolonchocarpin, I-80066

$C_{20}H_{18}O_4$
Abyssinone I, A-80006
3,4-Dibenzoyl-2,5-hexanedione, D-60081
4′-Hydroxyisolonchocarpin, *in* I-80066
Neorautenol, N-80023
4,5-Phenanthrenedimethanol; Di-Ac, *in* P-60070

$C_{20}H_{18}O_5$
Canescacarpin, *in* G-80029
Crotalarin, C-60171
6-(1,1-Dimethyl-2-propenyl)-4′,5,7-trihydroxyisoflavone, D-80472
Glyceollin III, G-80029
1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, *in* C-80165
Moracin *H*, *in* M-60145
Wighteone, W-80002

$C_{20}H_{18}O_6$
Ambonone, *in* N-80025
1″,2″-Dehydrocyclokievitone, D-80021
2,3-Dehydrokievitone, *in* K-80010
1,2-Diacetoxy-5,6-dimethoxyphenanthrene, *in* T-60115
Erythrinin C, E-80054
Fremontin, F-80080
Garveatin *A* quinone, G-60006
Licoisoflavone A, L-80028
Nepseudin, N-80025
Platanetin, P-70105
3′,4′,5,7-Tetrahydroxy-8-prenylflavone, T-80116

$C_{20}H_{18}O_7$
6-Desmethoxyhormothamnione, *in* H-50127
Meridinol, M-80033

$C_{20}H_{18}O_8$
Arborone, A-60294
Di-*p*-toluoyl tartrate, *in* T-70005
Moluccanin, M-70151
5,5′,6,7-Tetramethoxy-3′,4′-methylenedioxyflavone, *in* H-70081
3′,4′,5,5′-Tetramethoxy-6,7-methylenedioxyisoflavone, *in* H-80071

$C_{20}H_{18}O_9$
2′-Acetoxy-5,5′-dihydroxy-3,7,8-trimethoxyflavone, *in* H-70080
Cetraric acid, C-70035
7-Hydroxy-5,5′,6,8-tetramethoxy-3′,4′-methylenedioxyflavone, *in* H-80029

$C_{20}H_{18}O_{10}$
Conphysodalic acid, C-60162

$C_{20}H_{19}Br$
Bromododecahedrane, B-80202

$C_{20}H_{19}Cl$
Chlorododecahedrane, C-80055

$C_{20}H_{19}ClO_7$
4′-Chloronephroarctin, *in* N-70032

$C_{20}H_{19}F$
Fluorododecahedrane, F-80033

$C_{20}H_{19}N$
2*H*-Dibenz[*e,g*]isoindole; *N-tert*-Butyl, *in* D-70067

$C_{20}H_{19}NO_3$
Dodecahedranol; *O*-Nitrate, *in* D-80523

$C_{20}H_{19}N_3$
▷ Rosaniline, R-60010

$C_{20}H_{20}$
1,1′-Bitetralinylidene, B-70165
▷ 7,12-Dimethylbenz[*a*]anthracene; 1,2,3,4-Tetrahydro, *in* D-60405
Dodecahedrane, D-60514

$C_{20}H_{20}O$
Dodecahedranol, D-80523

$C_{20}H_{20}O_3$
Asnipyrone B, A-80178
1-(3,4-Dihydroxyphenyl)-5-(4-hydroxyphenyl)-1-penten-4-yne, D-80365
Eupomatenoid 4, *in* E-60075

$C_{20}H_{20}O_4$
Abyssinone II, A-80007
Crotmadine, C-80157
Dehydroguaiaretic acid, D-80025
Desmethylxanthohumol, *in* I-80100
Eupomatenoid 7, *in* E-60075
Fruticulin *A*, F-60076
Glabranin, G-70015
Glabridin, G-70016
Licarin E, L-80026
Moracin *I*, *in* M-60146
Phaseollidin, P-80076
Psorolactone, P-60188
Pygmaeocine *E*, P-70144

$C_{20}H_{20}O_5$
Anastomosine, A-80154
Aphyllodenticulide, A-70243
5-Deoxykievitone, *in* K-80010
7,8-(2,2-Dimethylpyrano)-3,4′,5-trihydroxyflavan, D-60448
Glyceollidin I, G-80027
Glyceollidin II, G-80028
Helikrausichalcone, H-80007
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one; 4′-*O*-(3-Methyl-2-butenyl), *in* H-80246
10-Isopentenylemodinanthran-10-ol, I-60111
Machilin *B*, M-60002
Moracin *J*, *in* M-60146
Sandwicarpin, *in* C-80156
4′,5,7-Trihydroxy-3′-prenylflavanone, T-80334
Zuonin *A*, Z-60003

$C_{20}H_{20}O_6$
Cardiophyllidin, C-70023
5,6-Didehydropygmaeocin A, *in* P-80195
2-Hydroxygarveatin *A*, *in* H-60148
Kievitone, K-80010
O^5-Methyl-3′,4′-deoxypsorospermin-3′-ol, *in* D-60021
Rhynchosperin *A*, R-60007
Sigmoidin *B*, S-70041
Vittagraciliolide, V-70017

$C_{20}H_{20}O_7$
Juglorin, J-70005
Nephroarctin, N-70032
2′,3′,4′,5,6-Pentamethoxyflavone, *in* P-70030
2′,3,5,7,8-Pentamethoxyflavone, *in* P-70029
3,4′,5,6,7-Pentamethoxyflavone, *in* P-80035
3,5,6,7,8-Pentamethoxyflavone, *in* P-70031
2′,4′,5,5′,7-Pentamethoxyisoflavone, *in* P-80041
2′,4′,5′,6,7-Pentamethoxyisoflavone, *in* P-80042
3′,4′,5′,6,7-Pentamethoxyisoflavone, *in* P-80044
3′,4′,5,7,8-Pentamethoxyisoflavone, *in* P-80045
Rhynchosperin *B*, *in* R-60007
Sigmoidin *D*, S-60031

$C_{20}H_{20}O_8$
4′-Hydroxy-3,3′,5,6,7-pentamethoxyflavone, *in* H-80067
5-Hydroxy-3,3′,4′,6,7-pentamethoxyflavone, *in* H-80067
6-Hydroxy-2′,3,5,5′,7-pentamethoxyflavone, *in* H-60064
7-Hydroxy-3,3′,4′,5,6-pentamethoxyflavone, *in* H-80067

$C_{20}H_{20}O_9$
3,5-Dihydroxy-3′,4′,5′,7,8-pentamethoxyflavone, *in* H-70021
3′,5-Dihydroxy-4′,5′,6,7,8-pentamethoxyflavone, *in* H-80029
5,7-Dihydroxy-3,3′,4′,5′,8-pentamethoxyflavone, *in* H-70021
5,7-Dihydroxy-3′,4′,5′,6,8-pentamethoxyflavone, *in* H-80029

$C_{20}H_{20}O_{10}$
4′,5,5′,7-Tetrahydroxy-2′,3,6,8-tetramethoxyflavone, *in* O-60022
3′,5,7-Trihydroxy-3,4′,5′,6,8-pentamethoxyflavone, *in* O-70018
3′,5,7-Trihydroxy-3,4′,5′,6,8-pentamethoxyflavone, *in* O-70018
4′,5,5′-Trihydroxy-2′,3,6,7,8-pentamethoxyflavone, *in* O-60022
4′,5,7-Trihydroxy-2′,3,5′,6,8-pentamethoxyflavone, *in* O-60022
4′,5,7-Trihydroxy-3,3′,5′,6,8-pentamethoxyflavone, *in* O-70018
1,3,7-Trihydroxyxanthone; 3-Me ether, 7-glucoside, *in* T-80347

$C_{20}H_{20}O_{11}$
3,3′,4′,5,7-Pentahydroxyflavanone; 3-*O*-β-D-Xylopyranoside, *in* P-70027
1,3,5,8-Tetrahydroxyxanthone; 3-Me ether, 8-glucoside, *in* T-70123

$C_{20}H_{21}ClO_7$
Methyl eriodermate, *in* E-70032

$C_{20}H_{21}N$
Aminododecahedrane, A-80071

$C_{20}H_{22}$
2,5-Dimethyl-3,4-diphenyl-2,4-hexadiene, D-60419

$C_{20}H_{22}ClNO_2$
Fontonamide, F-60067

$C_{20}H_{22}N_2O_4$
1,4-Dibenzyl-6,7-dihydroxy-1,4-diazocane-5,8-dione, D-80078

$C_{20}H_{22}O_2$
2-Cyclohexene-1,4-diol; Dibenzyl ether, *in* C-80181
3,3-Dimethyl-5,5-diphenyl-4-pentenoic acid; Me ester, *in* D-60420

$C_{20}H_{22}O_4$
Austrobailignan-5, A-70270
Bibenzyl-2,2′-dicarboxylic acid; Di-Et ester, *in* B-80071
Dehydrodieugenol, D-80023
Dehydrodieugenol B, D-80024
6-(3-Methyl-2-butenyl)allopteroxylin, *in* A-60075
Phaseollidinisoflavan, P-80077

$C_{20}H_{22}O_5$
Austrobailignan-7, A-70271
Bacchotricuneatin B, B-80006
Ethuliacoumarin, E-60045
Fragransin E_1, *in* A-70271
2-Hydroxygarveatin *B*, H-60148
Phyllnirurin, P-80142
3,4′,5,7-Tetrahydroxy-8-prenylflavan, T-60125
Volkensiachromone, V-60016

$C_{20}H_{22}O_6$
Acuminatin, A-60062
Bartemidiolide, B-70008
Columbin, C-60160
2,3-Dehydroteucrin *E*, *in* T-60180
2-Deoxychamaedroxide, *in* C-60032
2,3-Dihydroxy-2,3-diphenylbutanedioic acid; Di-Et ester, *in* D-80312
12-Epiteuscordonin, *in* T-80165
2-Hydroxyligustrin; 2-Ketone, 8-O-(2-methyl-2,3-epoxybutanoyl), *in* H-80184
Isobutyrylshikonin, *in* S-70038
Ligustrin; 8-*O*-(2,5-Dihydro-5-hydroxy-3-furancarboxylate), *in* L-80030
Ligustrin; $\Delta^{1(10)}$-Isomer, 8-*O*-(2,5-dihydro-5-hydroxy-3-furancarboxylate), *in* L-80030
8*β*-(2-methyl-2,3-epoxybutyroyloxy)-dehydroleucodin, *in* H-80184
1-(2,3,4,5,6-Pentamethoxyphenyl)-3-phenyl-2-propen-1-one, *in* P-80050
Pygmaeocin A, P-80195
Teuscorodonin, T-80165

$C_{20}H_{22}O_7$
Chamaedroxide, C-60032
2-Dehydroarcangelisinol, D-70021
Desacylisoelephantopin senecioate, *in* I-60099
Desacylisoelephantopin tiglate, *in* I-60099
10α-Hydroxycolumbin, *in* C-60160
8*β*-Hydroxycolumbin, *in* C-60160
1-Hydroxypinoresinol, H-60221
9-Hydroxypinoresinol, H-70216
Isojateorin, *in* C-60160
Jateorin, *in* C-60160
2′,3′,4′,5,7-Pentamethoxyisoflavanone, *in* P-80039
Wikstromol, W-70003

$C_{20}H_{22}O_8$
Arizonin C_3, A-70255
2-Dehydroarcangelisinol; 2*β*,3*β*-Epoxide, 6,12-diepimer, *in* D-70021
6-Hydroxyarcangelisin, *in* D-70021
4′-Hydroxy-3′,5,5′,6,7-pentamethoxyflavone, *in* H-70081
Tinospora clerodane, T-70200

$C_{20}H_{22}O_9$
Afzelechin; 7-*O*-*β*-D-Apioside, *in* T-60104
Astringin, *in* D-80361
Salireposide, *in* D-70287
Viscutin 3, *in* T-60103

$C_{20}H_{22}O_{10}$
Polydine, *in* P-70026

$C_{20}H_{22}O_{13}$
MP-2, *in* H-80196

$C_{20}H_{23}NO_5$
Fuligorubin *A*, F-60079

$C_{20}H_{24}$
Nonacyclo[10.8.0.0^{2,11}.0^{4,9}.0^{4,19}.0^{6,17}.0^{7,16}.0^{9,14}.0^{14,19}]icosane, N-70070

$C_{20}H_{24}O_2$
Saprorthoquinone, S-80010

$C_{20}H_{24}O_3$
Centrolobin, C-80032
2-Epijatrogrossidione, *in* J-70002
Gravelliferone; Me ether, *in* G-60037
Jatrogrossidione, J-70002
Rubifolide, R-60016

$C_{20}H_{24}O_4$
Austrobailignan-6, A-60320
Bharangin, B-70088
Brayleanin, *in* C-60026
Coralloidolide *A*, C-60164
3,6-Dioxo-4,7,11,15-cembratetraen-10,20-olide, D-60470
12,16-Epoxy-11,14-dihydroxy-5,8,11,13-abietatetraen-7-one, E-60011
Gelomulide D, *in* G-80008
7-Geranyloxy-6-methoxycoumarin, *in* H-80189
Gersemolide, G-60015
Gersolide, G-60016
Gravelliferone; 8-Methoxy, *in* G-60037
Guaiaretic acid, G-70033
Hebeclinolide, H-60009
Isobharangin, I-80048
Polemannone, P-60166
Sirutekkone, S-70048
Vernoflexin, *in* Z-60001
Zaluzanin *C*; Angeloyl, *in* Z-60001

$C_{20}H_{24}O_5$
2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol, A-80046
1,11-Bisepicaniojane, *in* C-70013
Caniojane, C-70013
Epoxylaphodione, *in* D-60470
Ferulide, F-70005
3*β*-Hydroxyhebeclinolide, *in* H-60009
4-Hydroxyisobacchasmacranone, H-60161
Ligustrin; 8-*O*-(4-Hydroxytigloyl), *in* L-80030
Lycoxanthol, L-70046
Machilin *C*, M-60003
Machilin *D*, *in* M-60003
Machilin *I*, M-70003
Myristargenol *A*, M-70163
Myrocin *C*, M-70165
Nectandrin *B*, *in* M-70003
ent-7-Oxo-3,13-clerodadiene-16,15:18,19-olide, *in* H-80143

$C_{20}H_{24}O_6$
ent-2α-Acetoxy-7-oxo-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
Bacchariolide *B*, B-70004
Deacetylsessein, *in* S-60027
Deacetylteupyrenone, *in* T-60184
8-Deacyl-15-deoxypunctatin; 8-*O*-(2-Methyl-2,3-epoxybutanoyl), *in* D-80006
15-Deoxyliscundin, *in* D-80006
5-Desoxyeuparotin, *in* E-80090
Heliopsolide, H-70007
2-Hydroxyligustrin; 8-*O*-(2-methyl-2,3-epoxybutanoyl), *in* H-80184
ent-Isolariciresinol, *in* I-60139
Isolariciresinol, *in* I-60139
Isotaxiresinol; 7-Me ether, *in* I-60139
Ladibranolide, L-60008
Lariciresinol, L-70019
Methyl 12,17;15,16-diepoxy-6-hydroxy-19-nor-17-oxo-4,13(16),14-clerodatrien-18-oate, M-80068
3,3′,4′,5,7-Pentamethoxyflavan, *in* P-70026
Sanguinone *A*, S-60006
Teucrin *E*, T-60180
Teucrin H2, *in* T-60180

$C_{20}H_{24}O_7$
Bacchariolide *A*, *in* B-70004
8-Deacyl-15-deoxypunctatin; 2α,3α-Epoxy, 8-*O*-(2-hydroxymethyl-2*Z*-butenoyl), *in* D-80006
8-Deacyl-15-deoxypunctatin; 2α,3α-Epoxy, 8-*O*-(2-methyl-2,3-epoxybutanoyl), *in* D-80006
Euparotin, E-80090
1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxy-1-propenyl)-2-methoxyphenoxy]-1,3-propanediol, H-80193
Liscundin, *in* D-80006
Melampodin *D*, M-60013
Orthopappolide methacrylate, *in* O-60045
Punctaliatrin, *in* D-80006
Tomenphantopin *A*, *in* T-60222
Zinaflorin IV, Z-80002
Zinaflorin IV; O^6-Deacyl, O^6-tigloyl, *in* Z-80002

$C_{20}H_{24}O_8$
4*β*,15-Epoxy-1*β*-methoxy-9*Z*-*millerenolide*, *in* M-60137
15-Hydroxy-3-dehydrotifruticin, *in* T-80197

$C_{20}H_{24}O_{10}$
Salicortin, S-70002

$C_{20}H_{24}O_{13}$
Diospyroside, *in* D-84287

$C_{20}H_{24}S_6$
2,3,11,12-Dibenzo-1,4,7,10,13,16-hexathia-2,11-cyclooctadecadiene, D-60073

$C_{20}H_{26}O_2$
12-Hydroxy-6,8,11,13-abietatrien-3-one, H-80105

$C_{20}H_{26}O_3$
19(4→3)-Abeo-11,12-dihydroxy-4(18),8,11,13-abietatetraen-7-one, A-60003
ent-15-Beyerene-2,3,12-trione, *in* D-80285
6,7-Dehydroroyleanone, *in* R-60015
11,12-Dihydroxy-5,8,11,13-abietatetraen-7-one, D-80266
10-Epinidoresedic acid, *in* N-70035
12-Hydroxy-8,11,13-abietatriene-3,7-dione, H-80103
12-Hydroxy-8,11,13-abietatriene-6,7-dione, H-80104
3-(2-Hydroxy-4,8-dimethyl-3,7-nonadienyl)benzaldehyde; Ac, *in* H-60122
Kahweol, K-60002
Methyl *p*-geranyloxycinnamate, *in* H-80242
Nidoresedic acid, N-70035
ent-6-Oxo-7,12*E*,14-labdatrien-17,11α-olide, O-60076
Strictic acid, S-70077

$C_{20}H_{26}O_4$
19(4*β*→3*β*)-Abeo-6,11-epoxy-6,12-dihydroxy-6,7-seco-4(18),8,11,13-abietatetraen-7-al, A-60004
Anisomelic acid, A-60275
Citlalitrione, C-80135
Cynajapogenin *A*, C-70257
Desoxyarticulin, *in* A-60307
Dihydroguaiaretic acid, *in* G-70033
11,12-Dihydroxy-6,8,11,13-abietatetraen-20-oic acid, D-60305
5,12-Dihydroxy-6,8,12-abietatriene-11,14-dione, D-80267
6,12-Dihydroxy-8,11,13-abietatriene-1,7-dione, D-80268
2α,11-Dihydroxy-7,9(11),13-abietatriene-6,12-dione, *in* D-70282
ent-7*β*,14α-Dihydroxy-1,16-kauradiene-3,15-dione, D-80324
ent-3*β*,14α-Dihydroxy-7,9(11),15-pimaratriene-2,12-dione, D-80373
ent-8α,14α-Epoxy-3*β*-hydroxy-9(11),15-pimaradiene-2,12-dione, E-80032
ent-8*β*,14*β*-Epoxy-3*β*-hydroxy-9(11),15-pimaradiene-2,12-dione, *in* E-80032
15,16-Epoxy-12-oxo-8(17),13(16),14-labdatrien-19-oic acid, *in* L-60011
Gelomulide C, G-80008
Hardwickiic acid; 19-Oxo, *in* H-70002
4-Hydroxysapriparaquinone, H-80254
17-Oxohebemacrophyllide, *in* H-60010
11,12,16-Trihydroxy-5,8,11,13-abietatetraen-7-one, T-60312

$C_{20}H_{26}O_5$
Articulin, A-60307
Ballotinone, *in* M-70013
Chapinolin, C-70037
Cumambranolide; 8α-Angeloyloxy, *in* C-80164
Cumambranolide; 8β-Angeloyloxy, *in* C-80164
Cumambranolide; 8α-Tigloyloxy, *in* C-80164
8,9-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide; 9-(2*R*,3*R*-Epoxy-2-methylbutanoyl), *in* D-60323
11,12-Dihydroxy-7-oxo-8,11,13-abietatrien-20-oic acid, *in* T-60337
Epirosmanol, *in* R-70010
Feruginin, F-60004
Gibberellin A_{24}, G-60019
Gibberellin A_{64}, G-70012
7-Hydroxy-3,13-clerodadiene-16,15;18,19-diolide, H-70116
ent-2α-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide, H-80142
ent-7β-Hydroxy-3,13-clerodadiene-15,16;18,19-diolide, H-70117
ent-7β-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide, H-80143
ent-7α-Hydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80143
Mollisorin *A*, *in* D-70302
Myristargenol *B*, M-70164
ent-7-Oxo-3-clerodene-15,16:18,19-diolide, *in* H-70117
Peregrinone, *in* M-70013
Rosmanol, R-70010
Senecioodontol, S-60022
Spongialactone A, S-80043
2,6,7,11-Tetrahydroxy-5,7,9(11),13-abietatetraen-12-one, T-80085
Thymifodioic acid, T-60218
11,12,14-Trihydroxy-8,11,13-abietatriene-3,7-dione, T-60313

$C_{20}H_{26}O_6$
Caleine *F*, *in* C-60005
Candesalvone B, C-80015
Coleon *C*, C-60157
Coralloidolide *B*, C-60165
Cumambranolide; 8β-(Epoxyangeloyloxy), *in* C-80164
Cumambranolide; 8β-(3-Hydroxy-2-methylenebutanoyloxy), *in* C-80164
Cumambranolide; 8β-Sarracinoyloxy, *in* C-80164
Deacetyleupaserrin, *in* D-70302
Deoxytifruticin, *in* T-80197
ent-2α,7β-Dihydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
2,8-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide; 8-(3*S*-Hydroxy-2-methylenebutanoyl), *in* D-70302
4,5-Epoxy-2,8-dihydroxy-1(10),11(13)-germacradien-12,6-olide; 8-(3-Methyl-2-butenoyl), *in* E-60013
Gibberellin A_{36}, *in* G-60019
Gibberellin A_{65}, G-70013
Gigantanolide *A*, *in* T-60323
Gigantanolide *B*, *in* T-60323
Jurinelloide, J-60003
Mollisorin *B*, *in* D-70302
Sesebrinic acid, S-60026
Teulamifin *B*, T-70158
Teumicropin, T-60181
7,11,12-Trihydroxy-6-oxo-8,11,13-abietatrien-20-oic acid, T-60337
Zoapatanolide *B*, Z-70007

$C_{20}H_{26}O_7$
Cyclocratystyolide, C-70216
2,8-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide; 8-(2*R*,3*R*-Epoxy-2-hydroxymethylbutanoyl), *in* D-70302
Gibberellin A_{66}, *in* G-70013
20-Hydroxyelemajurinelloide, H-60132
20-Hydroxyjurinelloide, *in* J-60003
Specionin, S-70059
Tifruticin, T-80197

$C_{20}H_{26}O_8$
8-Deacyltrichogoniolide; 8-*O*-Angeloyl, *in* D-80007
Specionin, S-60039

$C_{20}H_{26}O_9$
8β-Propionyloxy-10β-hydroxyhirsutinolide-13-*O*-acetate, *in* H-80089

$C_{20}H_{26}O_{10}$
Anamarine, A-60270

$C_{20}H_{27}ClO_7$
Lacinolide B, L-80016

$C_{20}H_{28}$
Hexacyclo[11.3.1.1^{3,7}.1^{5,9}.1^{11,15}.0^{2,10}]eicos-2-ene, H-70031

$C_{20}H_{28}N_2O_3$
Oxyphencyclimine, O-60102

$C_{20}H_{28}N_2O_8$
N-(*N*-1-Carboxy-6-hydroxy-3-oxoheptyl)alanyltyrosine, C-70022

$C_{20}H_{28}O$
8,11,13-Abietatrien-12,16-oxide, A-60008
Biadamantylidene epoxide, B-70091
8,11,13-Cleistanthatrien-19-al, *in* C-60154

$C_{20}H_{28}O_2$
6,8,11,13-Abietatriene-2,12-diol, A-80003
ent-16-Atisene-3,14-dione, A-80185
Barbatusol, B-60007
ent-15-Beyerene-2,12-dione, B-80065
ent-15-Beyerene-3,12-dione, *in* D-80285
Cedronellone, C-60027
3,7,11,15(17)-Cembratetraen-16,2-olide, C-60028
8,11,13-Cleistanthatrien-19-oic acid, *in* C-60154
10(20),16-Ericacadien-19-oic acid, E-80050
12-Ethyl-13-methoxy-8,11,13-podocarpatrien-7-one, *in* N-80030
12-Hydroxy-8,11,13-abietatrien-18-al, *in* A-70005
ent-2-Hydroxy-1,15-beyeradien-3-one, H-80115
11-Hydroxy-8,11,13-cleistanthatrien-7-one, H-80141
Nimbonolone, N-80030
Nimbosone, N-80031
ent-8(14),15-Pimaradiene-3,12-dione, *in* P-80146
Taonianone, T-60006
Totarolone, *in* T-70204

$C_{20}H_{28}O_3$
6,8,11,13-Abietatetraene-11,12,14-triol, A-60006
Antiquorin, A-80166
Bacchabolivic acid, B-80004
12,15-Dihydroxy-8,11,13-abietatrien-7-one, D-80270
2,11-Dihydroxy-7,9(11),13-abietatrien-12-one, D-70282
2,12-Dihydroxy-8,11,13-abietatrien-7-one, D-70281
3,12-Dihydroxy-8,11,13-abietatrien-1-one, D-60306
6,14-Dihydroxy-8,11,13-abietatrien-1-one, D-80271
Hardwickiic acid, H-70002
Hebemacrophyllide, H-60010
ent-3β-Hydroxy-15-beyerene-2,12-dione, *in* D-80285
14-Hydroxy-8,12-cleistanthadiene-7,11-dione, H-80140
6-Hydroxy-5-oxo-7,15-fusicoccadien-15-al, H-60203
19-Hydroxy-13(16),14-spongiadien-3-one, H-70220
Isolobophytolide, I-60106
Lambertianic acid, L-60011
7-Oxo-8(14),15-isopimaradien-18-oic acid, O-70094
ent-15-Oxo-16-kauren-18-oic acid, O-60075
ent-15-Oxo-16-kauren-18-oic acid, O-80086
ent-13R-hydroxy-16-atisene-3,14-dione, *in* A-80185
Royleanone, R-60015
Wedeliasecokaurenolide, W-60004

$C_{20}H_{28}O_4$
2α-Angeloyloxy-9-oxoisoanhydrooplopanone, *in* O-50045
Brevifloralactone, B-70179
Candesalvone A, C-80014
Curculathyrane *A*, C-60176
Curculathyrane *B*, C-60177
Demethylpinusolide, *in* P-60156
15,16-Dihydro-16-oxohardwickiic acid, *in* H-70002
7,12-Dihydroxy-8,12-abietadiene-11,14-dione, D-80265
2β,12-Dihydroxy-8,12-abietadiene-11,14-dione, *in* R-60015
11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid, D-80269
7,15-Dihydroxy-8,11,13-abietatrien-18-oic acid, D-70280
3,10-Dihydroxy-5,11-dielmenthadiene-4,9-dione, D-60316
ent-3α,11α-Dihydroxy-16-kaurene-6,15-dione, D-80325
ent-13*R*-14*R*-Dihydroxy-3-oxo-15-atisen-17-al, D-80349
3,19-Dihydroxy-13(16),14-spongiadien-2-one, D-70345
2α,19-Dihydroxy-13(16),14-spongiadien-3-one, *in* H-70220
Ephemeric acid, E-60006
6,11-Epoxy-6,12-dihydroxy-6,7-seco-8,11,13-abietatrien-7-al, E-60014
ent-15,16-Epoxy-4α-hydroxy-13(16),14-clerodadiene-3,12-dione, E-80029
Furanopetasin, *in* F-70047
Grayanotoxin XX, *in* G-80040
Gutiesolbriolide, G-80045
Hautriwaic acid, *in* H-70002
2β-Hydroxyhardwickiic acid, *in* H-70002
17-Hydroxyhebemacrophyllide, *in* H-60010
Isogutiesolbriolide, I-80062
Isospongiadiol, I-60137
Ivangustin; *O*-(2-Methylbutanoyl), *in* I-70109
Kerlinic acid, K-70011
Marrubiin, M-70013
Patagonic acid, P-70013
Pseudopterogorgia diterpenoid *C*, P-70129
3,11,12-Trihydroxy-8,11,13-abietatrien-7-one, T-60314
ent-7β,14α,15β-Trihydroxy-1,16-kauradien-3-one, T-80312

$C_{20}H_{28}O_5$
8,9-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide; 8-(2-Methylbutanoyl), *in* D-60323
11,12-Epoxy-2,14-dihydroxy-5,8(17)-briaradien-18,7-olide, E-70012
ent-7β,20-Epoxy-1β,14α,20-trihydroxy-16-kauren-15-one, E-80046
Gutiesolbriolide; 17-Hydroxy, 10E-isomer, *in* G-80045
ent-7β-Hydroxy-3-clerodene-15,16:18,19-diolide, *in* H-70117
17-Hydroxygutiesolbriolide, *in* G-80045
2-Hydroxyhautriwaic acid, *in* H-70002
17-Hydroxyisogutiesolbriolide, *in* I-80062
16-Hydroxy-8(17),13-labdadien-15,16-olid-19-oic acid, H-80182
Longikaurin *A*, L-70035
Melisodoric acid, M-70018
Pulchellin 2-*O*-tiglate, *in* P-80189
2α,6α,7,11-Tetrahydroxy-7,9(11),13-abietatrien-12-one, *in* D-70282
ent-1β,3α,11α-Trihydroxy-16-kaurene-6,15-dione, T-80313
ent-1β,7β,14α-Trihydroxy-16-kaurene-3,15-dione, T-80314
ent-7β,12β,14α-Trihydroxy-16-kaurene-3,15-dione, T-80315
2,11,12-Trihydroxy-6,7-seco-8,11,13-abietatriene-6,7-dial 11,6-hemiacetal, T-80339

$C_{20}H_{28}O_6$
Amarolide, A-60085
Blumealactone *A*, *in* B-70172
Blumealactone *B*, *in* B-70172
Gigantanolide *C*, *in* T-60323
6α-Hydroxypulchellin 4-*O*-angelate, *in* P-80189
Schkuhridin *A*, *in* S-60012
Sigmoidin *A*, *in* S-70041

6,7,12,16-Tetrahydroxy-8,12-abietadiene-11,14-dione, T-80084
ent-1β,3α,7α,11α-Tetrahydroxy-16-kaurene-6,15-dione, T-60109

$C_{20}H_{28}O_7S$
2,8-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide; 8-(2*S*-Hydroxy-2-hydroxymethyl-3*S*-mercaptobutanoyl), *in* D-70302

$C_{20}H_{28}O_{10}$
Ptelatoside *B*, *in* H-70209

$C_{20}H_{30}$
Pentaisopropylidenecyclopentane, P-60053

$C_{20}H_{30}O$
8,11,13-Abietatrien-19-ol, A-60007
8,11,13-Abietatrien-3-ol, A-70006
8,11,13-Cleistanthatrien-19-ol, C-60154
ent-15,16-Epoxy-7,13(16),14-labdatriene, E-70022
8(14),15-Isopimaradien-3-one, I-80076
8(17),13(16),14-Labdatrien-19-al, *in* L-80010
Mikanifuran, M-70148
Totarol, T-70204

$C_{20}H_{30}O_2$
Abeoanticopalic acid, A-60002
8(14),13(15)-Abietadien-18-oic acid, A-80001
8,11,13-Abietatriene-12,18-diol, A-70005
ent-15-Beyeren-18-oic acid, B-80066
13,15-Cleistanthadien-18-oic acid, A-60317
Cycloanticopalic acid, C-60181
Dictyodial *A*, D-70145
5,8,11,14,16-Eicosapentaenoic acid, E-80009
15,16-Epoxy-8-isopimaren-7-one, E-80033
3,4-Epoxy-13(15),16,18-sphenolobatrien-5-ol, E-60031
ent-3-Hydroxy-15-beyeren-2-one, H-80116
ent-3β-Hydroxy-15-beyeren-12-one, *in* D-80285
18-Hydroxy-8,15-isopimaradien-7-one, H-60162
ent-12β-Hydroxy-8(14),15-pimaradien-3-one, *in* P-80146
ent-3β-Hydroxy-8(14),15-pimaradien-12-one, *in* P-80146
8,15-Isopimaradien-18-oic acid, I-80073
ent-9βH-Isopimara-7,15-dien-17-oic acid, *in* I-80075
Isosarcophytoxide, I-70100
ent-16*S*-Kaurane-17,19-dial, *in* K-70008
ent-15-Kauren-17-oic acid, K-60008
ent-15-Kauren-18-oic acid, K-80009
8(17),12-Labdadiene-15,16-diol, L-80002
8(17),13(16),14-Labdatrien-19-oic acid, L-80010
ent-2-Oxo-7,13-labdadien-15-al, *in* D-80328
Perrottetianal *A*, P-60064
ent-9(11),15-Pimaradien-19-oic acid, P-80147
Reiswigin *B*, *in* R-60004
Sanadaol, S-70008
Sandaracopimaric acid, S-80008
Sarcophytoxide, S-70011
3,7,11,15-Tetramethyl-13-oxo-2,6,10,14-hexadecatetraenal, T-60150

$C_{20}H_{30}O_3$
8,11,13-Abietatriene-7,18-diol, A-70004
Agroskerin, A-70076
Agrostistachin, A-60067
Agrostistachin, A-80041
2α-Angeloxyanhydrooplopanone, *in* O-50045
Ascidiatrienolide A, A-80176
Ascidiatrienolide B, *in* A-80176
Ascidiatrienolide C, *in* A-80176
ent-3β,4β;15,16-Diepoxy-13(16),14-clerodadien-2β-ol, D-80153
ent-3β,16α-Dihydroxy-13-atisen-2-one, D-80272
ent-2α,3β-Dihydroxy-15-beyeren-12-one, D-80285
ent-3β,12α-Dihydroxy-15-beyeren-2-one, D-80286
ent-3β,12β-Dihydroxy-15-beyeren-2-one, *in* D-80286
1-(2,6-Dihydroxyphenyl)-4-methyl-4-tridecen-1-one, D-80368
ent-3β,12β-Dihydroxy-8(14),15-pimaradien-2-one, *in* P-80146
ent-3α,4α-Epoxy-13-cleroden-15,16-olide, E-80019
5,6-Epoxy-7,9,11,14-eicosatetraenoic acid, E-60015
ent-15,16-Epoxy-2β-hydroxy-13(16),14-clerodadien-3-one, *in* E-80016
15,16-Epoxy-11β-hydroxy-8-isopimaren-7-one, *in* E-80033
14,15-Epoxy-8(17),12-labdadien-16-oic acid, E-60025
15,16-Epoxy-13,17-spatadiene-5,19-diol, E-60029
2-(2-Formyl-3-hydroxymethyl-2-cyclopentenyl)-6,10-dimethyl-5,9-undecadienal, F-70038
Grayanotoxin XIX, *in* G-80040
2-[(2,3,3*a*,4,5,7*a*-Hexahydro-3,6-dimethyl-2-benzofuranyl)ethylidene]-6-methyl-5-heptenoic acid, H-60050
2-[(3,4,4*a*,5,6,8*a*-Hexahydro-4,7-dimethyl-2*H*-1-benzopyran-2-yl)ethylidene]-6-methyl-5-heptenoic acid, H-60046
ent-18-Hydroxy-15-beyeren-19-oic acid, H-60106
ent-7α-Hydroxy-15-beyeren-19-oic acid, H-60104
ent-12β-Hydroxy-15-beyeren-19-oic acid, H-60105
7-Hydroxy-13(17),15-cleistanthadien-18-oic acid, H-70115
16-Hydroxy-3,13-clerodadien-15,16-olide, H-70118
ent-2α-Hydroxy-3,13-clerodadien-15,16-olide, H-80145
Hydroxydictyodial, *in* D-70145
8-Hydroxy-5,9,11,14,17-eicosapentaenoic acid, H-70126
6α-Hydroxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
7α-Hydroxyisopimara-8(14)15-dien-18-oic acid, *in* S-80008
12β-Hydroxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
3β-Hydroxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
ent-1α-Hydroxy-16-kauren-19-oic acid, H-80179
ent-12β-Hydroxy-15-kauren-19-oic acid, H-80180
ent-3β-Hydroxy-15-kauren-17-oic acid, H-60167
ent-3β-Hydroxy-16-kauren-18-oic acid, H-80181
13*R*-Hydroxy-8,14-labdadiene-2,7-dione, *in* D-80327
ent-3β-Hydroxy-2-oxo-7,13-labdadien-15-al, *in* D-80328
Isosarcophytoxide; 3,4-Epoxide, *in* I-70100
Medigenin, M-70015
Naviculide, N-80016
6-Oxo-3,13-clerodadien-15-oic acid, O-70081
ent-2-oxo-3,13-clerodadien-15-oic acid, *in* C-80142
ent-2-Oxo-3,13-clerodadien-15-oic acid, *in* H-80144
5-Oxo-6,8,11,14-eicosatetraenoic acid, O-80080
ent-15-Oxo-1(10),13-halimadien-18-oic acid, O-60069
2-Oxokolavenic acid, *in* K-60013
7-Oxo-8,13-labdadien-15-oic acid, O-70095
16-Oxo-17-spongianal, O-60094

$C_{20}H_{30}O_4$
8(14)-Abieten-18-oic acid 9,13-endoperoxide, A-60009
β-Cyclohallerin, *in* C-60193
α-Cyclohallerin, C-60193
Cymbodiacetal, C-60233
ent-3β,19-Dihydroxy-15-kauren-17-oic acid, D-60341
ent-3β,18-Dihydroxy-19-trachylobanoic acid, D-80388
*r*1(10)13E-*Halimadiene*-15,18-*dioic acid*diedie, *in* O-60069
-1(10),13Z-*Halimadiene*-15,18-*dioic acid*enien, *in* O-60069
ent-3α,4α-Epoxy-2α-hydroxy-13-cleroden-15,16-olide, *in* E-80019
ent-3α,4α-Epoxy-16ξ-hydroxy-13-cleroden-15,16-olide, *in* E-80019
14,15-Epoxy-5-hydroxy-6,8,10,12-eicosatetraenoic acid, E-70016
▷ Grayanotoxin VII, G-80040
Grayanotoxin VIII, *in* G-80040
Hydroxyagrostistachin, *in* A-80041
17-Hydroxy-15,17-oxido-16-spongianone, H-60201
ent-4α-Hydroxy-3-oxo-13-cleroden-15,16-olide, *in* D-80303
Isohallerin, I-60100
Kurubashic acid angelate, *in* K-60014
Lapidin, *in* L-60014
Neohalicholactone, *in* H-80002
Paniculadiol, P-80007
Phlogantholide *A*, P-70099
ent-3α,7β,14α-Trihydroxy-16-kauren-15-one, T-60326
ent-1β,7β,14*S*-Trihydroxy-16-kauren-15-one, T-50476

$C_{20}H_{30}O_5$
6,17-Dihydroxy-15,17-oxido-16-spongianone, D-60365
1β,10α-Epoxykurubashic acid angelate, *in* K-60014
ent-9,13-Epoxy-7-labdene-15,17-dioic acid, E-70024
Ivangustin; 4,5α-Dihydro,4α-hydroxy, O^1-(2-methylbutanoyl), *in* I-70109
6-Oxo-7-labdene-15,17-dioic acid, O-60077
ent-3α,7β,14α,20-Tetrahydroxy-16-kauren-15-one, T-60110
ent-7β,11α,14*S*,20-Tetrahydroxy-16-kauren-15-one, T-70115
ent-1β,7β,14*S*,20-Tetrahydroxy-16-kauren-15-one, T-70114
ent-7α,18,19-Trihydroxy-3,13-clerodadien-16,15-olide, T-80291
5,14,15-Trihydroxy-6,8,10,12,17-eicosapentaenoic acid, T-70256
5,6,15-Trihydroxy-7,9,11,13,17-eicosapentaenoic acid, T-70255
ent-7α,9α,15β-Trihydroxy-16-kauren-19-oic acid, T-80316

$C_{20}H_{30}O_5S$
Umbraculumin *B*, U-70002

$C_{20}H_{30}O_6$
Grayanotoxin XVII, *in* G-80039
6β-Hydroxypulchellin 2-*O*-isovalerate, *in* P-80189
Ingol, I-70018
Maoecrystal K, M-80008
ent-2α,3α,6β,7β,11β-Pentahydroxy-16-kauren-15-one, P-80047
ent-1β,3α,6β,7α,11α-Pentahydroxy-16-kauren-15-one, P-80048
Phlebiakauranol aldehyde, P-70097
3,4,6,8-Tetrahydroxy-11,13-clerodadien-15,16-olide, T-70103

$C_{20}H_{30}O_7S$
Hymatoxin *A*, H-60235

$C_{20}H_{30}O_8$
▷ Ptaquiloside, P-60190

$C_{20}H_{30}S_2$
Di(2-adamantyl) disulfide, *in* A-80038

$C_{20}H_{31}BrO$
Sphaeroxetane, S-70061

$C_{20}H_{31}BrO_3$
15-Bromo-9(11)-parguerene-2,7,16-triol, B-80241

$C_{20}H_{31}BrO_4$
15-Bromo-9(11)-parguerene-2,7,16,19-tetrol, B-80240

$C_{20}H_{31}NO_5S$
Latrunculin *D*, L-50032

$C_{20}H_{32}$
Bicyclo[8.8.2]eicosa-1(19),10(20),19-triene, B-70096
α-Camphorene, C-70009

Cycloaraneosene, C-80170
Dictytriene *A*, D-70148
Dictytriene *B*, *in* D-70148
1,5-Dimethyl-8-(5-methyl-1-methylene-4-hexenyl)-1,5-cyclodecadiene, D-80453
Isosphaerodiene 1, I-80091
Isosphaerodiene 2, *in* I-80091
Laurenene, L-60018
Ruzicka's hydrocarbon, R-80017

$C_{20}H_{32}Br_2O_2$
12-Hydroxybromosphaerol, H-60108

$C_{20}H_{32}N_2O_3S$
▷ Carbosulfan, C-80022

$C_{20}H_{32}O$
7,13-Abietadien-18-ol, A-80002
1,3,7,11-Cembratetraen-15-ol, C-70029
Dictymal, D-60162
8β-Hydroxycycloaraneosene, *in* C-80170
8(14),15-Isopimaradien-18-ol, I-80074
ent-9β*H*-Isopimara-7,15-dien-17-ol, I-80075
ent-16*S*-Kauran-17-al, K-70008
ent-11-Kaurene-16β,18-diol, K-60006
ent-16-Kauren-3β-ol, K-70010
Neodolabellenol, N-70022
Neodolabellenol; 5-Epimer, *in* N-70022
18-Oxo-3-virgene, O-60095
ent-9,(11),15-Pimaradien-19-ol, P-80148
Rotalin A, R-80012
13,17-Spatadien-10-ol, S-70058
Sphaeropyrane, S-70060
3,7,11,15-Tetramethyl-2,6,10,13,15-hexadecapentaen-1-ol, T-70137
ent-3β-Trachylobanol, T-80205
1(15),8(19)-Trinervitadien-9-ol, T-70300

$C_{20}H_{32}O_2$
ent-15-Beyerene-14β,19-diol, B-80064
1(14),4,8,12-Cembratetraene-2,3-diol, C-80030
Cladiellin; Δ^3-Isomer, *O*-de-Ac, *in* C-80137
ent-4(18),-13-Clerodadien-15-oic acid, C-80142
ent-2,4(18),13-Clerodatriene-15,16-diol, C-80143
Dictyone, D-70146
Dilophic acid, D-60394
ent-11α,16α-Epoxy-17-kauranol, E-80034
8,13-Epoxy-14-labden-11-one, E-80037
14,15-Epoxy-3,7,11,15-tetramethyl-2,6,10-hexadecatrienal, E-80045
ent-19-Hydroxy-16*S*-kauran-17-al, *in* K-70008
15-Hydroxy-8(17),12-labdadien-16-al, H-70145
19-Hydroxy-8(17),13-labdadien-15-al, H-70146
ent-15-Hydroxy-7,13-labdadien-2-one, *in* L-80004
ent-15-Hydroxy-8,13-labdadien-7-one, *in* L-70004
12-Isoagathen-15-oic acid, I-60085
7,15-Isopimaradiene-18,19-diol, I-70078
7,15-Isopimaradiene-3,18-diol, I-70076
7,15-Isopimaradiene-3,19-diol, I-70077
8(14),15-Isopimaradiene-2,18-diol, I-60113
8(14),15-Isopimaradiene-3,18-diol, I-70080
8(14),15-Isopimaradiene-3,18-diol, I-80069
8,15-Isopimaradiene-7,18-diol, I-70079
ent-16*R*-Kauran-17-oic acid, *in* K-70008
ent-16*S*-Kauran-17-oic acid, *in* K-70008
16-Kaurene-3,13-diol, K-80007
ent-16-Kaurene-7α,15β-diol, K-70009
ent-15-Kaurene-3β,17-diol, K-60007
Kolavenic acid, K-60013
ent-7,12*E*,14-Labdatriene-6β,17-diol, L-60004
ent-8(14),15-Pimaradiene-3β,12β-diol, P-80146
Reiswigin *A*, R-60004
Stemodinone, *in* S-70071
1(15),8(19)-Trinervitadiene-2,3-diol, T-70295
13*R*-*Hydroxy*-8(17),14-*labdadien*-3-*one*, *in* L-70002

$C_{20}H_{32}O_3$
6β-Angeloyloxy-1α-hydroxy-5,10-bisepi-4(15)-eudesmene, *in* E-80084
Dehydroplexaurolone, *in* P-80163
Dictyotriol *A*, D-70147
ent-16α,17-Dihydroxy-3-atisanone, D-70284
3,15-Dihydroxy-8(17),13-labdadien-19-al, D-70310
2,13-Dihydroxy-8,14-labdadien-7-one, D-80327
ent-3β,15-Dihydroxy-7,13-labdadien-2-one, D-80328
1-(2,6-Dihydroxyphenyl)-1-tetradecanone, D-70338
Epivittadinal, *in* V-70016
ent-4α,18-Epoxy-13-cleroden-15-oic acid, *in* C-80142
ent-4β,18-Epoxy-13-cleroden-15-oic acid, *in* C-80142
11,12-Epoxy-5,8,14-eicosatrienoic acid, E-60017
8,9-Epoxy-5,11,14-eicosatrienoic acid, E-60016
8α,13*R*-Epoxy-6β-hydroxy-14-labden-11-one, *in* E-80037
3,4-Epoxy-13(15),16-sphenolobadiene-5,18-diol, E-60030
2,3,4,7,8,8*a*-Hexahydro-8-(5-hydroxy-4-methylpentyl)-6,8-dimethyl-1*H*-3*a*,7-methanoazulene-3-carboxylic acid, H-70057
ent-16α-Hydroxy-18-atisanoic acid, *in* A-80184
ent-2α-Hydroxy-3,13-clerodadien-15-oic acid, H-80144
12-Hydroxy-5,8,10,14-eicosatetraenoic acid, H-60131
5-Hydroxy-6,8,11,14-eicosatetraenoic acid, H-60127
8-Hydroxy-5,9,11,14-eicosatetraenoic acid, H-60128
12-Hydroxy-6-(hydroxymethyl)-10-methyl-2-(4-methyl-3-pentenyl)-2,6,10-dodecatrienal, *in* H-70179
11-Hydroxy-5,8,12,14-icosatetraenoic acid, H-60130
9-Hydroxy-5,7,11,14-icosatetraenoic acid, H-60129
8-Hydroxy-5,9,11,14-icosatetraenoic acid, *in* H-70126
2-Hydroxy-8(17),13-labdadien-15-oic acid, H-70147
ent-6β-Hydroxy-8(17),13-labdadien-15-oic acid, H-70148
2-(6-Hydroxy-4-methyl-4-hexenylidene)-6,10-dimethyl-7-oxo-9-undecenal, H-60186
12-Hydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenoic acid, H-70223
16-Hydroxy-2,6,10,14-tetramethyl-2,6,10,14-hexadecatetraenoic acid, H-70224
Isodehydroplexaurolone, *in* P-80163
7,15-Isopimaradiene-2,3,19-triol, I-70081
8(14),15-Isopimaradiene-2,18,19-triol, I-80071
8(14),15-Isopimaradiene-3,18,19-triol, I-80072
8,15-Isopimaradiene-3,7,19-triol, I-70082
ent-7,11*E*,14-Labdatriene-6β,13ξ,17-triol, L-60005
Pilosanone *A*, P-60153
ent-5-Rosene-3α,15,16,18-tetrol, *in* R-60011
11,15(17)-Trinervitadiene-3,9,13-triol, T-70297
1(15),8(19)-Trinervitadiene-2,3,20-triol, T-70299
1(15),8(19)-Trinervitadiene-2,3,9-triol, T-70298
Vittadinal, V-70016

$C_{20}H_{32}O_4$
15-Angeloyloxy-10-hydroxy-4-oplopanone, *in* D-80348
Cervicol, C-70034
Chatferin, *in* F-60009
ent-3β,4α-Dihydroxy-13-cleroden-15,16-olide, D-80303
1,18-Dihydroxy-14-decipien-19-oic acid, D-80311
12,19-Dihydroxy-5,8,10,14-eicosatetraenoic acid, D-60319
15,20-Dihydroxy-5,8,11,13-eicosatetraenoic acid, D-70297
5,20-Dihydroxy-6,8,11,14-eicosatetraenoic acid, D-70296
5,6-Dihydroxy-7,9,11,14-eicosatetraenoic acid, D-80313
ent-13,16-Dihydroxy-8(17),14-labdadien-18-oic acid, D-80326
3,6-Dihydroxy-2-(1-oxo-10-tetradecenyl)-2-cyclohexen-1-one, D-70332
ent-15,16-Epoxy-13(16),14-clerodadiene-2β,3β,4α-triol, E-80016
14,15-Epoxy-20-hydroxy-5,8,11-eicosatrienoic acid, E-70018
5,6-Epoxy-20-hydroxy-8,11,14-eicosatrienoic acid, E-70017
9,13-Epoxy-7,14-labdadiene-2,3,20-triol, E-80035
Grayanotoxin XVIII, G-80041
Halicholactone, H-80002
10-Hydroxy-2-(6-hydroxy-4-methyl-4-hexylidene)-6,10-dimethyl-7-oxo-8-undecenal, *in* H-60186
8(14),15-Isopimaradiene-2,3,18,19-tetrol, I-80070
7-Labdene-15,17-dioic acid, L-60006
7-Labdene-15,17-dioic acid, L-80011
7-Labdene-15,18-dioic acid, L-60007
Oliveric acid, O-60039
Pilosanone *B*, *in* P-60153
Salvicin, S-60003
Stolonidiol, S-60055
ent-2α,3α,16-Trihydroxy-8(14)-pimaren-15-one, *in* P-60154
1(15),8(19)-Trinervitadiene-2,3,9,20-tetrol, T-70296

$C_{20}H_{32}O_5$
Camporic acid, C-70010
11,15-Dihydroxy-9-oxo-5,13-prostadienoic acid, D-60367
8α,13*R*-Epoxy-6β,7β,9-trihydroxy-14-labden-11-one, *in* E-80037
▷ Grayanotoxin II, G-80038
Grayanotoxin VI, *in* G-80040
ent-16-Kaurene-1β,3α,6β,11α,15α-pentol, K-80008
Methyl 3,6-epidioxy-6-methoxy-4,14,16-octadecatrienoate, *in* E-60008
Pulchellin 2-*O*-isovalerate, *in* P-80189
Sterebin *B*, *in* S-60052
Sterebin *C*, *in* S-60052
Tetradecahydro-4,6-dihydroxy-9,9,12*a*-trimethyl-6*H*-phenanthro[1,10*a*-*c*]furan-3-carboxylic acid, T-60038
ent-3β,4α,16ξ-Trihydroxy-13-cleroden-15,16-olide, *in* D-80303
5,14,15-Trihydroxy-6,8,10,12-eicosatetraenoic acid, T-60320
3,7,11-Trimethyl-2,6,10-dodecatrienoic acid; 2-Acetoxy-3-hydroxypropyl ester, *in* T-60364

$C_{20}H_{32}O_6$
8,13-Epoxy-1,6,7,9-tetrahydroxy-14-labden-11-one, E-70027
Grayanotoxin V, *in* G-80039
Grayanotoxin XI, *in* G-80038
Grayanotoxin XII, *in* G-80038
Laserol, *in* L-60016
Nardostachin, N-70019
Phlebiakauranol alcohol, *in* P-70097

$C_{20}H_{32}O_7$
8,19-Epoxy-1(15)-trinervitene-2,3,7,9,14,17-hexol, E-80048

$C_{20}H_{32}O_8$
Odonticin, O-80026

$C_{20}H_{33}BrO_2$
Bromotetrasphaerol, B-70272
Rotalin B, R-80013

$C_{20}H_{34}BrClO_2$
Dactylomelol, D-80001

$C_{20}H_{34}N_6O_2$
3,9,17,23,29,30-Hexaaza-6,20-dioxatricyclo[23.3.1.1^{11,15}]triaconta-1(28),11(29),12,14,25,27-hexaene, H-80036

$C_{20}H_{34}O$
13-Epi-5β-neoverrucosanol, *in* N-70030
13-Epi-5β-neoverrucosanol, *in* N-80024
8,13-Epoxy-14-labdene, E-70023
Helipterol, H-80009
5-Homoverrucosanol, H-80095
8-Hydroxyisopimar-15-ene, H-60163
8(17),12-Labdadien-3-ol, L-70012
5-Neoverrucosanol, N-80024
Neoverrucosanol, N-70030
Obscuronatin, O-60002
Tormesol, T-80203

$C_{20}H_{34}O_2$
ent-16α,18-Atisanediol, A-80184

2,7,11-Cembratriene-4,6-diol, C-80031
Chromophycadiol, C-60148
ent-4(18)-Cleroden-15-oic acid, *in* C-80142
3,7-Dolabelladiene-6,12-diol, D-70541
ent-16-Hydroxy-13-epimanoyl oxide, *in* E-70023
12α-Hydroxy-13-epi-manoyl oxide, *in* E-70023
8-Hydroxy-13-labden-15-al, H-70149
15-Hydroxy-7-labden-3-one, H-70151
19-Hydroxymanoyl oxide, *in* E-70023
7,14-Labdadiene-3,13-diol, L-80001
8(17),13-Labdadiene-3,15-diol, L-70001
8(17),14-Labdadiene-3,13-diol, L-70002
ent-8,13(16)-Labdadiene-14,15-diol, L-70005
ent-7,13-Labdadiene-2α,15-diol, L-80003
ent-7,14-Labdadiene-2α,13-diol, L-70003
ent-8,13-Labdadiene-7α,15-diol, L-70004
ent-8(17),13-Labdadiene-7α,15-diol, L-70006
ent-8(17),13-Labdadiene-9α,15-diol, L-70007
ent-7,13-Labdadiene-2β,15-diol, L-80004
ent-7,13*E*-Labdadiene-3β,15-diol, L-60001
ent-8,13-Labdadiene-7β,15-diol, *in* L-70004
Secomanool, S-80017
Stemodin, S-70071

$C_{20}H_{34}O_3$
ent-3β,16α,17-Atisanetriol, A-70266
7,11-Bis(hydroxymethyl)-3,15-dimethyl-2,6,10,14-hexadecatetraen-1-ol, B-80151
ent-3,13-Clerodadiene-15,16,17-triol, C-80141
Dictytriol, *in* D-70148
8,15-Dihydroxy-13-labden-19-al, D-70311
3β,15-Dihydroxy-8-labden-7-one, *in* L-70013
7,8-Epoxy-2,11-cembradiene-4,6-diol, E-60010
ent-3α,4α-Epoxy-15-clerodanoic acid, E-80018
ent-4α,18-Epoxy-15-clerodanoic acid, *in* C-80142
ent-4β,18-Epoxy-15-clerodanoic acid, *in* C-80142
Gypopinifolone, G-70036
ent-4β-Hydroxy-13-cleroden-15-oic acid, *in* C-80142
15-Hydroxy-8(17)-labden-19-al, H-70150
15-Hydroxy-7-labden-17-oic acid, H-60168
15-Hydroxy-7-labden-17-oic acid, H-80183
6-(Hydroxymethyl)-10-methyl-2-(4-methyl-3-pentenyl)-2,6,10-dodecatriene-1,12-diol, H-70179
ent-15-Hydroxy-8,9-seco-13-labdene-8,9-dione, H-70218
Isodictytriol, *in* D-70148
3,13,16-Kauranetriol, K-80005
ent-2α,16β,17-Kauranetriol, K-60004
ent-7α,16β,18-Kauranetriol, K-80006
ent-3β,16β,17-Kauranetriol, K-60005
8,13-Labdadiene-6,7,15-triol, L-60003
ent-7,14-Labdadiene-2α,13,20-triol, L-70011
ent-7,14-Labdadiene-2α,3α,13-triol, L-70010
ent-7,13-Labdadiene-2β,3β,15-triol, L-80009
Pachytriol, P-70001
Plexaurolone, P-80163
ent-5-Rosene-15,16,19-triol, R-60012
ent-5-Rosene-15,16,18-triol, *in* R-60012
Vinigrol, V-70009

$C_{20}H_{34}O_4$
6,15-Dihydroxy-7-labden-17-oic acid, D-60342
6,15-Dihydroxy-8-labden-17-oic acid, D-80329
7,15-Dihydroxy-8-labden-17-oic acid, D-80330
1(15)-Dolastene-4,8,9,14-tetrol, D-70543
6,13-Epoxy-3-eunicellene-8,9,12-triol, E-80027
Jewenol A, J-70003
Jewenol B, J-70004
11,13-Labdadiene-6,7,8,15-tetrol, L-70009
7,14-Labdadiene-2,3,13,20-tetrol, L-80007
8,13-Labdadiene-2,6,7,15-tetrol, L-60002
8(17),14-Labdadiene-2,7,13,20-tetrol, L-80008
ent-8(14)-Pimarene-2α,3α,15*R*,16-tetrol, P-60154
ent-5-Rosene-3α,15,16,19-tetrol, R-60011
ent-2β,15,16-Trihydroxy-13-cleroden-3-one, T-80292

$C_{20}H_{34}O_5$
8,20-Epoxy-14-labdene-2,3,7,13-tetrol, E-80036
4(15)-Eudesmen-11-ol; α-L-Arabopyranoside, *in* E-70066
11,13(16)-Labdadiene-6,7,8,14,15-pentol, L-70008
8,14-Labdadiene-2,3,7,13,20-pentol, L-80005
8(17),14-Labdadiene-2,3,7,13,20-pentol, L-80006
Methyl 3,6-epidioxy-6-methoxy-4,16-octadecadienoate, *in* E-60008
Sterebin *H*, *in* L-70008
Tucumanoic acid, T-60410

$C_{20}H_{34}O_6$
▷ Grayanotoxin III, G-80039

$C_{20}H_{35}BrO_3$
Venustanol, V-70004

$C_{20}H_{36}$
Tetra-*tert*-butylcyclobutadiene, T-70014
Tetra-*tert*-butyltetrahedrane, T-70015

$C_{20}H_{36}Cl_2O_{10}$
7(18),11(19)-Havannadichlorohydrin, H-70005

$C_{20}H_{36}N_4O_8$
1,5,9,13-Tetraazacyclohexadecane-1,5,9,13-tetraacetic acid, T-60016

$C_{20}H_{36}O$
2,2-Di-*tert*-butyl-3-(di-*tert*-butylmethylene)cyclopropanone, D-70101
ent-14-Labden-8β-ol, L-70014

$C_{20}H_{36}O_2$
13-Episclareol, *in* S-70018
8,13-Epoxy-3-labdanol, E-70021
7-Labdene-15,17-diol, L-80012
8(20)-Labdene-3,15-diol, L-80013
Peucelinendiol, P-80075
Sclareol, S-70018

$C_{20}H_{36}O_3$
Dihydroplexaurolone, *in* P-80163
ent-3α,4α-Epoxy-13,15-clerodanediol, E-80017
8-Labdene-3,7,15-triol, L-70013
7-Pimarene-3,15,16-triol, P-80149

$C_{20}H_{36}O_4$
ent-8,13-Epoxy-14,15,19-labdanetriol, E-70020
3-Hydroxymethyl-7,11,15-trimethyl-2,6,10-hexadecatriene-1,14,15-triol, H-80215

$C_{20}H_{36}O_5$
ent-13-Clerodene-2β,3β,4α,15,16-pentol, C-80144
Methyl 3,6-epidioxy-6-methoxy-4-octadecenoate, *in* E-60008
ent-2β,3β,4α-Trihydroxy-15-clerodanoic acid, *in* T-60410
9,12,13-Trihydroxy-10,15-octadecadienoic acid, T-80327

$C_{20}H_{36}S$
2,3-Dimethyl-5-(2,6,10-trimethylundecyl)thiophene, D-70446

$C_{20}H_{37}NO_3$
N-(Tetrahydro-2-oxo-3-furanyl)hexadecanamide, *in* A-60138

$C_{20}H_{38}O$
3,7,11,15-Tetramethyl-2-hexadecenal, *in* P-60152

$C_{20}H_{38}O_3$
11,15-Epoxy-3(20)-phytene-1,2-diol, E-80043
Gyplure, *in* O-60006

$C_{20}H_{38}O_5$
9*S*,12*S*,13*S*-Trihydroxy-10*E*-octadecenoic acid, *in* T-80327

$C_{20}H_{40}$
3-Icosene, I-80003

$C_{20}H_{40}Br_2$
1,20-Dibromoicosane, D-70092

$C_{20}H_{40}O$
Phytol, P-60152

$C_{20}H_{40}O_2$
7,11,15-Trimethyl-3-methylene-1,2-hexadecanediol, T-60368

$C_{20}H_{40}O_3$
19-Hydroxyicosanoic acid, H-80176

$C_{20}H_{42}O$
2-Icosanol, I-80002

$C_{20}H_{50}N_{10}$
1,4,7,10,13,16,19,22,25,28-Decaazacyclotriacontane, D-70011

$C_{21}H_{11}F_5O_3$
9-Fluorenylmethyl pentafluorophenyl carbonate, F-60019

$C_{21}H_{12}N_4$
▷ Tricycloquinazoline, T-60271

$C_{21}H_{12}N_6$
[1,3,5]Triazino[1,2-*a*:3,4-*a'*:5,6-*a''*]trisbenzimidazole, T-60238

$C_{21}H_{12}O_2$
7*H*-Dibenzo[*c*,*h*]xanthen-7-one, D-60080

$C_{21}H_{13}N$
Phenanthro[9,10-*g*]isoquinoline, P-60075

$C_{21}H_{13}NO_2$
Dibenzo[*c*,*g*]carbazole-6-carboxylic acid, D-80068

$C_{21}H_{13}N_3OS$
12*H*-Quinoxalino[2,3-*b*][1,4]benzothiazine; *N*-Benzoyl, *in* Q-70008

$C_{21}H_{14}O$
2,3-Diphenyl-1*H*-inden-1-one, D-70482

$C_{21}H_{15}N$
1,2-Diphenyl-3-(phenylimino)cyclopropene, D-70491

$C_{21}H_{15}NO_2$
Dibenz[*b*,*g*]azocine-5,7(6*H*,12*H*)-dione; *N*-Ph, *in* D-60068

$C_{21}H_{15}O_2^{\oplus}$
2,4,5-Triphenyl-1,3-dioxol-1-ium, T-70307

$C_{21}H_{16}$
▷ 6-Methylcholanthrene, M-70056

$C_{21}H_{16}O_5$
Calopogonium isoflavone *B*, C-60006

$C_{21}H_{16}O_6$
Gerberinol 1, G-60013
Justicidin *B*, *in* D-60493

$C_{21}H_{16}O_7$
▷ Diphyllin, D-60493

$C_{21}H_{16}O_8$
1,3-Dihydroxy-2-hydroxymethylanthraquinone; Tri-Ac, *in* D-70306

$C_{21}H_{16}O_9$
Mitorubrinic acid, M-80192

$C_{21}H_{16}O_{11}$
α-Acetylconstictic acid, *in* C-60163

$C_{21}H_{18}N_2$
4,5-Dihydro-2,4,5-triphenyl-1*H*-imidazole, D-80263
Hydrobenzamide, H-80100

$C_{21}H_{18}O$
1,2,2-Triphenyl-1-propanone, T-60389
1,2,3-Triphenyl-1-propanone, T-60390
1,3,3-Triphenyl-1-propanone, T-60391
▷ 1,1,3-Triphenyl-2-propen-1-ol, T-70313

$C_{21}H_{18}O_3$
6-Methylene-2,4-cyclohexadien-1-one; Trimer, *in* M-60072

$C_{21}H_{18}O_4$
Calopogoniumisoflavone A, C-80013

$C_{21}H_{18}O_5$
Alpinumisoflavone; 4'-Me ether, *in* A-80050
Glabrachromene II, G-70014
Maximaisoflavone B, *in* H-80203
4'-*O*-Methylderrone, *in* D-80031
Neorautenane, *in* N-80022

$C_{21}H_{18}O_6$
Glycyrol, *in* P-80186

3′-Hydroxyalpinumisoflavone 4′-methyl ether, *in* A-80050
Isoglycyrol, I-80061
Neorautenanol, *in* N-80022
Pipoxide, P-60159
Racemoflavone, *in* A-80183

$C_{21}H_{18}O_7$
3-(2-Ethyl-2-butenyl)-9,10-dihydro-1,6,8-trihydroxy-9,10-dioxo-2-anthracenecarboxylic acid, E-70038
Hildecarpidin, H-60081

$C_{21}H_{18}O_{12}$
1,3,8,9-Tetrahydroxycoumestan; 3-*O*-Glucoside, *in* T-80087

$C_{21}H_{19}N$
Cyanododecahedrane, *in* D-80522

$C_{21}H_{19}NO$
1,3,3-Triphenyl-1-propanone; Oxime, *in* T-60391

$C_{21}H_{19}NO_5$
Isomurralonginol; 3-Pyridinecarboxylate, *in* I-70071

$C_{21}H_{20}$
Bicyclo[14.4.1]heneicosa-1,3,5,7,9,11,13,15,17,19-decaene, B-80077
Cyclopropadodecahedrane, C-80195

$C_{21}H_{20}O$
Dodecahedranecarboxaldehyde, D-80521

$C_{21}H_{20}O_2$
Dodecahedranecarboxylic acid, D-80522

$C_{21}H_{20}O_3$
Abbottin, A-70002

$C_{21}H_{20}O_5$
Edulenanol, *in* N-80023
Neorautane, N-80022
Pongachalcone II, P-80168

$C_{21}H_{20}O_6$
Angeloylprangeline, *in* P-60170
Aurmillone, *in* T-80113
Curcumin, C-80165
1-(3,4-Dimethoxyphenyl)-2,3-bis(hydroxymethyl)-6,7-methylenedioxynaphthalene, D-80414
Egonol; Ac, *in* E-70001
Garvin *B*, G-60009
Isoaurmillone, *in* T-80319
Kwakhurin, K-60016
Neorautanol, *in* N-80022
Topazolin, T-60224

$C_{21}H_{20}O_7$
Dehydrotrichostin, *in* T-70225
2-Hydroxygarvin *B*, *in* G-60009
Podoverine *A*, P-60164
Zeylenol, Z-70006

$C_{21}H_{20}O_8$
4′-Demethylpodophyllotoxin, *in* P-80165
4′,7-Dihydroxyisoflavone; 7-*O*-Rhamnoside, *in* D-80323
Homalicine, *in* H-70207
Hormothamnione, H-50127

$C_{21}H_{20}O_9$
Cleomiscosin *D*, C-70185
Daidzin, *in* D-80323
4′,6-Dihydroxyaurone; 6-*O*-β-D-Glucopyranosyl, *in* D-80273
4′,7-Dihydroxyisoflavone; 4′-*O*-β-D-Glucopyranoside, *in* D-80323
3,3′,4,5,8-Pentamethoxy-6,7-methylenedioxyflavone, *in* H-80028
Phenarctin, P-70054

$C_{21}H_{20}O_{10}$
Baptisin, *in* T-80110
Genistin, *in* T-80309
8-*C*-Glucosyl-4′,5,7-trihydroxyisoflavone, G-80025
Sophoricoside, *in* T-80309
2′,5,7-Trihydroxyisoflavone; 7-*O*-Glucoside, *in* T-80307

$C_{21}H_{20}O_{11}$
Aureusin, *in* A-80188
Cernuoside, *in* A-80188
8-*C*-Glucosyl-3′,4′,5,7-tetrahydroxyisoflavone, G-80024
Isoorientin, I-80068
Oroboside, *in* T-80109
Sulfurein, *in* S-70082

$C_{21}H_{20}O_{13}$
Quercetagitrin, *in* H-80067

$C_{21}H_{20}O_{14}$
Hibiscitin, *in* H-70021

$C_{21}H_{21}N$
2,2′,2″-Trimethyltriphenylamine, T-70288
3,3′,3″-Trimethyltriphenylamine, T-70289
4,4′,4″-Trimethyltriphenylamine, T-70290

$C_{21}H_{21}NO$
Dodecahedranecarboxylic acid; Amide, *in* D-80522

$C_{21}H_{21}N_3O_7$
Cacotheline, C-70001

$C_{21}H_{21}O_{10}^{\oplus}$
Callistephin, *in* T-80093
Fragarin, *in* T-80093
Pelargonenin, *in* T-80093
3,4′,5,7-Tetrahydroxyflavylium; 4′-Glucoside, *in* T-80093
3,4′,5,7-Tetrahydroxyflavylium; 7-Glucoside, *in* T-80093

$C_{21}H_{21}O_{11}^{\oplus}$
Columnin, *in* P-80037

$C_{21}H_{22}$
Des-A-26,27,28-trisnorursa-5,7,9,11,13,15,17-heptaene, D-80038

$C_{21}H_{22}O$
(Hydroxymethyl)dodecahedrane, H-80201

$C_{21}H_{22}O_3$
Asnipyrone A, A-80177

$C_{21}H_{22}O_4$
1,2-Diphenyl-1,2-cyclopropanedicarboxylic acid; Di-Et ester, *in* D-80509
Eupomatenoid 12, *in* E-60075
Isoxanthohumol/, I-80100
Kurospongin, K-70015
Sandwicensin, *in* P-80076
Tephrinone, *in* G-70015
Tephrobbottin, T-70007

$C_{21}H_{22}O_5$
Ambofuranol, A-80057
Aristotetralone, A-60298
Cristacarpin, C-80156
7,8-(2,2-Dimethylpyrano)-3,4′-dihydroxy-5-methoxyflavan, *in* D-60448
Garveatin *D*, G-60007
Helichromanochalcone, H-80005
Isoxanthohumol/, I-80099
Licobenzofuran, L-80027
3′-Methoxyglabridin, *in* G-70016
1-Methoxyphaseollidin, *in* P-80076
Pleurotin, P-80162
Quercetol *A*, Q-70001
3*a*,4,9,9*a*-Tetrahydro-9-(3,4,5-trimethoxyphenyl)naphtho[2,3-*c*]furan-1(3*H*)one, T-80080

$C_{21}H_{22}O_6$
O-Angeloylalkannin, *in* S-70038
β,β-Dimethylacrylalkannin, *in* S-70038
β,β-Dimethylacrylshikonin, *in* S-70038
2-Hydroxyaristotetralone, *in* A-70253
Sophoraisoflavanone A, *in* L-80028
4′,5,7-Trihydroxy-3′-methoxy-5′-prenylflavanone, *in* S-70041

$C_{21}H_{22}O_7$
Annulin *B*, A-60277
Divaronic acid, D-70528
Isopteryxin, *in* K-70013
Isosamidin, *in* K-70013
Praeruptorin *A*, P-60169
Pteryxin, *in* K-70013
▷ Samidin, *in* K-70013
Topazolin hydrate, *in* T-60224
Trichostin, T-70225

$C_{21}H_{22}O_8$
Dihydrohomalicine, *in* H-70207
Epoxypteryxin, *in* K-70013
3,3′,4′,5,6,7-Hexamethoxyflavone, *in* H-80067
3′,4′,5,5′,6,7-Hexamethoxyflavone, *in* H-70081
Isopseudocyphellarin *A*, I-70098
Pseudocyphellarin *A*, *in* P-70127

$C_{21}H_{22}O_9$
▷ Barbaloin, B-80010
3-Hydroxy-3′,4′,5,6,7,8-hexamethoxyflavone, *in* H-80028
3′-Hydroxy-4′,5,5′,6,7,8-hexamethoxyflavone, *in* H-80029
4′-Hydroxy-3′,5,5′,6,7,8-hexamethoxyflavone, *in* H-80029
5-Hydroxy-3,3′,4′,6,7,8-hexamethoxyflavone, *in* H-80028
5-Hydroxy-3′,4′,5′,6,7,8-hexamethoxyflavone, *in* H-80029
Isobarbaloin, *in* B-80010
Isoliquiritin, *in* D-80367
Neoisoliquiritin, *in* D-80367

$C_{21}H_{22}O_{10}$
Coreopsin, *in* D-80362
5,7-Dihydroxy-2′,3,4′,5′,6,8-hexamethoxyflavone, *in* O-60022
5,7-Dihydroxy-3,3′,4′,5′,6,8-hexamethoxyflavone, *in* O-70018
Isosalipurposide, *in* H-80246
Monospermoside, *in* D-80362

$C_{21}H_{22}O_{11}$
Pyracanthoside, *in* T-70105
Stillopsin, *in* D-70339

$C_{21}H_{22}O_{12}$
Astilbin, *in* P-70027
Glucodistylin, *in* P-70027
Isoglucodistylin; *in* P-70027
Lanceoside, *in* P-60052
Taxifolin 4′-glucoside, *in* P-70027
1,3,5,8-Tetrahydroxyxanthone; 3,5-Di-Me ether, 8-*O*-β-D-glucopyranoside, *in* T-70123

$C_{21}H_{23}ClO_7$
Methyl 2-*O*-methyleriodermate, *in* E-70032
Methyl 2′-*O*-methyleriodermate, *in* E-70032
Methyl 4-*O*-methyleriodermate, *in* E-70032

$C_{21}H_{24}O_3$
5-(3,5-Di-*tert*-butyl-4-oxo-2,5-cyclohexadienylidene)-3,6-cycloheptadiene-1,2-dione, D-70105

$C_{21}H_{24}O_4$
5-Deoxymyricanone, *in* M-70162
8-Geranyloxypsoralen, *in* X-60002
6-(3-Methyl-2-butenyl)allopteroxylin methyl ether, *in* A-60075
O-Methyldehydrodieugenol, *in* D-80023
2′-*O*-Methylphaseollidinisoflavan, *in* P-80077

$C_{21}H_{24}O_5$
Aristochilone, A-70251
Aristotetralol, A-70253
Calopiptin, *in* A-70271
α,α-Dimethylallylcyclolobin, *in* U-80002
8-(3,3-Dimethylallyl)-5-methoxy-3,4′,7-trihydroxyflavan, *in* T-60125
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*,3,4-*b*′]dipyran-2-one, *in* M-80001
5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *in* M-80001
4-(3-Hydroxy-3-methylbutanoyloxy)-3-(1,1-dimethyl-2-propenyl)-6-phenyl-2*H*-pyran-2-one, *in* D-70434
Machilin G, *in* A-70271
5-Methylethuliacoumarin, *in* E-60045
Myricanone, *in* M-70162
Obionin A, O-80001
Praealtin A, P-80172
Rutamarin, *in* C-60031

$C_{21}H_{24}O_6$
Arctigenin, A-70249
Penicillide, P-80019
Phillygenin, P-60141
▷ Phloridzin, *in* H-80244
Shikonin isobutyrate, *in* S-70038

$C_{21}H_{24}O_7$
Arnebin II, *in* D-80343
Dihydrosamidin, *in* K-70013
Dihydrotrichostin, D-70273
β-Hydroxyisovalerylshikonin, *in* S-70038
1-Hydroxypinoresinol; 4″-Me ether, *in* H-60221
Medioresinol, M-70016
Subsphaeric acid, S-80049
Suksdorfin, *in* K-70013
▷ Visnadin, *in* K-70013

$C_{21}H_{24}O_8$
Albaspidin AA, *in* A-80043
Aspidin AA, *in* A-80180
9α-Hydroxymedioresinol, *in* M-70016
Pseudocyphellarin *B*, P-70127

$C_{21}H_{24}O_9$
Glycyphyllin, *in* H-80244
Isorhapontin, *in* D-80361
Rhapontin, *in* D-80361

$C_{21}H_{24}O_{10}$
7,7*a*-Dihydro-3,6,7-trihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]oxiren-2(1*aH*)-one; 7-Ketone, 3-*O*-β-D-glucopyranoside, *in* D-70277

$C_{21}H_{26}O_3$
1,11-Bis(3-furanyl)-4,8-dimethyl-3,6,8-undecatrien-2-ol, B-70143
Malabaricone *A*, M-70007

$C_{21}H_{26}O_4$
1-(2,6-Dihydroxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone, *in* M-70007
15,20-Epoxy-3β-hydroxy-14,15-seco-5,15,17(20)-pregnatriene-2,14-dione, *in* A-70267
9-Phenyl-1-(2,4,6-trihydroxyphenyl)-1-nonanone, P-80138

$C_{21}H_{26}O_5$
Aristolignin, A-60297
5,7-Dihydroxy-7-(3-methyl-2-butenyl)-8-(2-methyl-2-oxopropyl)-3-propyl-2*H*-1-benzopyran-2-one, D-80340
1-(2,6-Dihydroxyphenyl)-9-(3,4-dihydroxyphenyl)-1-nonanone, *in* M-70007
3-*O*-Methyl-2,5-dehydrosenecioodentol, *in* S-60022
Myricanol, M-70162

$C_{21}H_{26}O_6$
Cordatin, C-60166
Fragransol *A*, F-70041
1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[2-methoxy-4-(1-propenyl)phenoxy]-1-propanol, *in* A-80046
Isolariciresinol 4′-methyl ether, *in* I-60139
Machilin *H*, M-70002
Subexpinnatin *B*, *in* S-60058

$C_{21}H_{26}O_7$
1-Ethoxy-9*Z*-*millerenolide*, *in* M-60137
Liriolignal, L-80035
Neocynaponogenin A, N-80019
Orthopappolide senecioate, *in* O-60045
Orthopappolide tiglate, *in* O-60045

$C_{21}H_{26}O_8$
Cratystyolide; Tri-Ac, *in* T-70257
4β,15-Epoxy-1β-ethoxy-4*Z*-*millerenolide*, *in* M-60137
Isorolandrolide, I-80087
8β-(2-Methylacryloyloxy)hirsutinolide 13-*O*-acetate, *in* H-80089

$C_{21}H_{26}O_9$
8-Deacyltrichogoniolide; 8-*O*-(2-Methylpropenoyl), 9-Ac, *in* D-80007
8β-(2-Hydroxymethylacryloyloxy)hisutinolide 13-*O*-acetate, *in* H-80089
Hypocretenoic acid; Lactone, 14-β-D-Glucopyranosyloxy, *in* H-70235
8β-(2-Methylacryloyloxy)-15-hydroxyhisutinolide 13-acetate, *in* H-80089
8β-(2-Methyl-2,3-epoxypropionyloxy)hirsutinolide 13-*O*-acetate, *in* H-80089

$C_{21}H_{26}O_{10}$
8β-Acetoxy-10β-hydroxyhirsutinolide 1,13-*O*-diacetate, *in* H-80089
8β,10β-Diacetoxyhirsutinolide 13-*O*-acetate, *in* H-80089
7,7*a*-Dihydro-3,6,7-trihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]oxiren-2(1*aH*)-one; 3-*O*-β-D-Glucopyranoside, *in* D-70277

$C_{21}H_{26}O_{13}$
Baisseoside, *in* D-84287

$C_{21}H_{27}ClO_{10}$
Tetragonolide, T-80053

$C_{21}H_{27}N_7O_{14}P_2$
▷ Coenzyme I, C-80145

$C_{21}H_{28}N_7O_{17}P_3$
Coenzyme II, C-80146

$C_{21}H_{28}O_2$
Avarone, *in* A-80189

$C_{21}H_{28}O_3$
12,13-Didehydrofurospongin I, *in* F-80097
1,3-Dioxototaryl methyl ether, *in* T-70204
Methyl nidoresedate, *in* N-70035

$C_{21}H_{28}O_4$
Atratogenin *A*, A-70267
Membranolide, M-60016
Smenoquinone, *in* I-80004
2,3,12-Trihydroxy-4,7,16-pregnatrien-20-one, T-60346

$C_{21}H_{28}O_5$
15,16-Dihydro-15-methoxy-16-oxonidoresedic acid, *in* N-70035
15,16-Dihydro-15-methoxy-16-oxostrictic acid, *in* S-70077
7-*O*-Formylhorminone, *in* D-80265
7-Methoxyrosmanol, *in* R-70010
3-*O*-Methylsenecioodentol, *in* S-60022

$C_{21}H_{28}O_7$
14-Acetoxy-9β-hydroxy-8β-(2-methylpropanoyloxy)-1(10),4,11(13)-germacratrien-12,6α-olide, *in* T-60323
Viguiestin, *in* T-70003

$C_{21}H_{28}O_8$
Vernoflexuoside, *in* Z-60001

$C_{21}H_{28}O_9$
Hypocretenoic acid; Lactone, 11α,13-Dihydro, 14-β-D-glucopyranosyloxy, *in* H-70235
Ixerin B, *in* I-80102
8-Propionoyloxy-10β-hydroxy-1-*O*-methylhirsutinolide-13-*O*-acetate, *in* H-80089

$C_{21}H_{29}BrO_4$
Bromovulone I, B-70278

$C_{21}H_{29}IO_4$
Iodovulone I, *in* B-70278

$C_{21}H_{29}NO_3$
Smenospongine, S-80036

$C_{21}H_{29}N_7O_{14}P_2$
Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 1,4-dihydro-1-β-D-ribofuranosyl-3-pyridinecarboxamide, *in* C-80145

$C_{21}H_{30}N_7O_{17}P_3$
NADPH, *in* C-80146

$C_{21}H_{30}O_2$
Avarol, A-80189

$C_{21}H_{30}O_3$
Furospongin I, F-80097
12-Methoxy-8,11,13-abietatrien-20-oic acid, M-60036
Methyl 7-oxo-8(14),15-isopimaradien-18-oate, *in* O-70094

$C_{21}H_{30}O_4$
7-*O*-Methylhorminone, *in* D-80265
Pinusolide, P-60156
2,3,12-Trihydroxy-4,7-pregnadien-20-one, T-60345

$C_{21}H_{30}O_5$
15,16-Dihydro-15-methoxy-16-oxohardwickiic acid, *in* H-70002
Kamebacetal *A*, K-70002
Kamebacetal *B*, *in* K-70002
Microglossic acid, M-60134
Spongionellin, S-60048
2,3,12,16-Tetrahydroxy-4,7-pregnadien-20-one, T-60124

$C_{21}H_{30}O_6$
4-Acetoxyflexilin, *in* F-70012
11-Dihydro-12-norneoquassin, D-60258

$C_{21}H_{30}O_7$
15-Desacetyltetraneurin *C* isobutyrate, *in* T-60158

$C_{21}H_{30}O_8$
Brachynereolide, B-60196
Macrocliniside G, *in* C-80164
Zaluzanin *C*; 11β,13-Dihydro, β-D-Glucoside, *in* Z-60001

$C_{21}H_{30}O_9$
11β,13-Dihydro-8α-hydroxyglucozaluzanin *C*, *in* Z-60001
Ixerin J, *in* I-80102

$C_{21}H_{30}O_{12}$
Cyclopropanehexacarboxylic acid; Hexa-Et ester, *in* C-70250

$C_{21}H_{30}O_{13}$
Acetylbarlerin, *in* S-60028

$C_{21}H_{30}Se$
Di-1-adamantyl selenoketone, D-70034

$C_{21}H_{31}N$
8-Isocyano-10,14-amphilectadiene, I-60090
7-Isocyano-11-cycloamphilectene, I-60094
7-Isocyano-1-cycloamphilectene, I-60093
8-Isocyano-1(12)-cycloamphilectrene, I-60095

$C_{21}H_{31}NO_5S$
Latrunculin *C*, *in* L-50032

$C_{21}H_{32}O_2$
1-(3,4-Methylenedioxyphenyl)-1-tetradecene, M-60077

$C_{21}H_{32}O_3$
ent-3β,4β;15,16-Diepoxy-2β-methoxy-13(16),14-clerodadiene, *in* D-80153
14-(3-Furanyl)-3,7,11-trimethyl-7,11-tetradecadienoic acid, F-70049
Gracilin *E*, *in* G-60035
Methyl 14ξ,15-epoxy-8(17),12*E*-labdadien-16-oate, *in* E-60025

$C_{21}H_{32}O_4$
Lycopersiconolide, L-60042

$C_{21}H_{32}O_5$
10,11-Dihydromicroglossic acid, *in* M-60134
Umbraculumin *A*, U-70001

$C_{21}H_{32}O_8$
11β,13-Dihydrobrachynereolide, *in* B-60196

$C_{21}H_{32}O_{10}$
Dihydroserruloside, D-70265
Ebuloside, E-60001

$C_{21}H_{32}O_{14}$
Aucubigenin; 1-*O*-β-Cellobioside, *in* A-80186
Aucubigenin; 1-*O*-β-Gentiobioside, *in* A-80186
10-Deoxymelittoside, *in* M-70019

$C_{21}H_{32}O_{15}$
Melittoside, M-70019

$C_{21}H_{33}N_3$
1,3,5-Tripiperidinobenzene, T-70314

$C_{21}H_{34}O_2$
Kolavenic acid; Me ester, *in* K-60013

$C_{21}H_{34}O_3$
15-Formylimbricatolal, *in* H-70150
12-Hydroxy-5,8,10,14-eicosatetraenoic acid; Me ester, *in* H-60131
5-Hydroxy-6,8,11,14-eicosatetraenoic acid; Me ester, *in* H-60127
8-Hydroxy-5,9,11,14-eicosatetraenoic acid; Me ester, *in* H-60128
11-Hydroxy-5,8,12,14-icosatetraenoic acid; Me ester, *in* H-60130
9-Hydroxy-5,7,11,14-icosatetraenoic acid; Me ester, *in* H-60129
1-(2-Hydroxy-6-methoxyphenyl)-1-tetradecanone, *in* D-70338

$C_{21}H_{34}O_4$
5,6-Dihydroxy-7,9,11,14-eicosatetraenoic acid; Me ester, *in* D-80313
ent-4α-Hydroxy-3β-methoxy-13-cleroden-15,16-olide, *in* D-80303

$C_{21}H_{34}O_5$
3,6-Epidioxy-6-methoxy-4,16,18-eicosatrienoic acid, E-60007

$C_{21}H_{34}O_6$
8,19-Epoxy-17-methyl-1(15)-trinervitene-2,3,7,9,14,17-hexol, E-80040

$C_{21}H_{34}O_{10}$
7,7-*O*-Dihydroebuloside, *in* E-60001

$C_{21}H_{34}O_{11}$
Patrinalloside, P-70014

$C_{21}H_{36}O_4$
15-Hydroxy-7α-methoxy-8-labden-17-oic acid, *in* D-80330

$C_{21}H_{36}O_5$
Arvoside, A-70264
Tetra-*tert*-butoxycyclopentadienone, T-70013

$C_{21}H_{36}O_7$
3-Eudesmene-1,6-diol; 6-*O*-β-D-Glucopyranoside, *in* E-80083

$C_{21}H_{36}O_8$
Methanetetrapropanoic acid; Tetra-Et ester, *in* M-70036

$C_{21}H_{38}O_3$
7α-Methoxy-8-labdene-3β,15-diol, *in* L-70013

$C_{21}H_{38}O_8$
Icariside C_1, *in* T-60362
Icariside C_2, *in* T-60362
Icariside C_3, *in* T-60362
Icariside C_4, *in* T-60362

$C_{21}H_{40}O_4$
Heneicosanedioic acid, H-80012

$C_{21}H_{42}O_2$
Heneicosanoic acid, H-80013

$C_{21}H_{42}O_3$
19-Hydroxyicosanoic acid; Me ester, *in* H-80176

$C_{21}H_{45}N_3O_3$
1,9,17-Trioxa-5,13,21-triazacyclotetracosane; 5,13,21-Tri-Me, *in* T-80358

$C_{22}H_{10}O_2$
10,11-Methano-1*H*-benzo[5,6]cycloocta[1,2,3,4-*def*]fluorene-1,14-dione, M-70039

$C_{22}H_{12}$
Benzo[*b*]benzo[3,4]cyclobuta[1,2-*h*]biphenylene, B-80015
Benzo[*h*]benzo[3,4]cyclobuta[1,2-*a*]biphenylene, B-80016
Benzo[*l*]cyclopenta[*cd*]pyrene, B-80018
Indeno[1,2,3-*cd*]fluoranthene, I-80010
▷ Indeno[1,2,3-*cd*]pyrene, I-70012

$C_{22}H_{12}N_2$
Dibenz[*b,h*]indeno[1,2,3-*de*][1,6]naphthyridine, D-60069
▷ Dibenzo[*c,f*]indeno[1,2,3-*ij*][2,7]naphthyridine, D-60074
2,2′-Diisocyano-1,1′-binaphthyl, D-60391

$C_{22}H_{12}N_2O$
Benzo[*a*]benzofuro[2,3-*c*]phenazine, *in* B-60033

$C_{22}H_{12}N_4$
Dibenzo[*cd*:*c′d′*][1,2,4,5]tetrazino[1,6-*a*:4,3-*a′*]diindole, D-60076

$C_{22}H_{12}O$
▷ Indeno[1,2,3-*cd*]pyren-1-ol, I-60022
▷ Indeno[1,2,3-*cd*]pyren-2-ol, I-60023
▷ Indeno[1,2,3-*cd*]pyren-6-ol, I-60024
▷ Indeno[1,2,3-*cd*]pyren-7-ol, I-60025
▷ Indeno[1,2,3-*cd*]pyren-8-ol, I-60026

$C_{22}H_{12}O_2$
Azuleno[1,2-*b*]anthracene-6,13-dione, A-80207

$C_{22}H_{12}O_9$
Pulviquinone A, P-80192

$C_{22}H_{12}S_2$
Naphtho[2,1-*b*:6,5-*b′*]bis[1]benzothiophene, N-60007

$C_{22}H_{13}N$
4*H*-Benzo[*def*]naphtho[2,3-*b*]carbazole, B-80024

$C_{22}H_{14}N_2$
Cycloocta[2,1-*b*:3,4-*b′*]diquinoline, C-70232

$C_{22}H_{14}O$
Benzo[*b*]triphenylen-10-ol, B-80050
Benzo[*b*]triphenylen-11-ol, B-80051
Benzo[*b*]triphenylen-1-ol, B-80046
Benzo[*b*]triphenylen-2-ol, B-80047
Benzo[*b*]triphenylen-3-ol, B-80048
Benzo[*b*]triphenylen-4-ol, B-80049
4,7:12,15-Diethenobenzo[7,8]cyclododeca[1,2-*c*]furan, D-80154

$C_{22}H_{14}O_2$
5,6:12,13-Diepoxy-5,6,12,13-tetrahydrodibenz[*a,h*]anthracene, D-70151

$C_{22}H_{14}O_3$
8,16-Epoxy-8*H*,16*H*-dinaphtho[2,1-*b*:2′,1′-*f*][1,5]dioxocin, E-70014

$C_{22}H_{14}O_4$
6,12-Dimethoxy-1,7-perylenedione, *in* D-80354
6,7-Dimethoxy-1,12-perylenedione, *in* D-80354

$C_{22}H_{14}O_6$
3,3′-Bi[5-hydroxy-2-methyl-1,4-naphthoquinone], B-60106

$C_{22}H_{14}O_9$
Aurintricarboxylic acid, A-60318

$C_{22}H_{15}F_3O_5S$
2,4,5-Triphenyl-1,3-dioxol-1-ium; Trifluoromethanesulfonate, *in* T-70307

$C_{22}H_{16}$
1,1:2,2-Bis([10]annulene-1,6-diyl)ethylene, B-70127
2,2-Di-(2-naphthyl)ethanal, D-80487
1,8-Diphenylnaphthalene, D-60483
Tribenzotriquinacene, T-80215

$C_{22}H_{16}O$
2,2-Di-(1-naphthyl)ethanal, D-80486
2-(1-Naphthyl)-2-(2-naphthyl)ethanal, N-80011

$C_{22}H_{16}O_2$
1,3-Diphenyl-1*H*-indene-2-carboxylic acid, D-60481

$C_{22}H_{16}O_6$
Dehydromillettone, *in* M-80191

$C_{22}H_{17}N$
3,5-Dihydro-4*H*-dinaphth[2,1-*c*:1′,2′-*e*]azepine, D-60234

$C_{22}H_{17}NO_2$
Dibenz[*b,g*]azocine-5,7(6*H*,12*H*)-dione; *N*-Benzyl, *in* D-60068

$C_{22}H_{17}N_7O_{13}S_2$
2,3-Bis(2-methoxy-4-nitro-5-sulfophenyl)-5-[(phenylamino)carbonyl]-2*H*-tetrazolium hydroxide inner salt, B-70151

$C_{22}H_{18}$
1,1,4-Triphenyl-1,3-butadiene, T-70305

$C_{22}H_{18}O$
1,1,1-Triphenyl-3-butyn-2-ol, T-80360

$C_{22}H_{18}O_2$
1,2-Di-2-naphthalenyl-1,2-ethanediol, D-80479

$C_{22}H_{18}O_3$
2-Hydroxy-1,3-diphenyl-1-propanone; Benzoyl, *in* H-70124

$C_{22}H_{18}O_6$
Durmillone, D-80537
Isojamaicin, I-80065
Millettone, M-80191

$C_{22}H_{18}O_7$
Justicidin *A*, *in* D-60493

$C_{22}H_{18}O_8$
Dehydropodophyllotoxin, *in* P-80165
Desertorin *A*, D-60022
2,4,5,6-Tetrahydroxyphenanthrene; Tetra-Ac, *in* T-60122

$C_{22}H_{18}O_{10}$
3-Galloylcatechin, *in* P-70026

$C_{22}H_{18}O_{14}$
Hexahydroxy-1,4-naphthoquinone; Hexa-Ac, *in* H-60065

$C_{22}H_{19}Br_2NO_3$
Deltamethrin, D-80027

$C_{22}H_{19}F_3O_2$
Dodecahedranol; Trifluoroacetyl, *in* D-80523

$C_{22}H_{20}$
3-(1,3,6-Cycloheptatrien-1-yl-2,4,6-cycloheptatrien-1-ylidenemethyl)-1,3,5-cycloheptatriene, C-60205
[2.2](4,7)(7,4)Indenophane, I-60021

$C_{22}H_{20}N_2O_2$
2,5-Dihydro-3,6-diphenylpyrrolo[3,4-*c*]pyrrole-1,4-dione; 2-Butyl, *in* D-70204
2,5-Dihydro-3,6-diphenylpyrrolo[3,4-*c*]pyrrole-1,4-dione; 2,5-Di-Et, *in* D-70204

$C_{22}H_{20}N_2S_2$
1,4-Bis(ethylthio)-3,6-diphenylpyrrolo[3,4-*c*]pyrrole, B-60158

$C_{22}H_{20}O_3$
1,1,2-Triphenyl-1,2-ethanediol; O^2-Ac, *in* T-70311

$C_{22}H_{20}O_4$
Caleprunifolin, C-80011
Erybraedin E, E-80052
Ethyl 2-ethoxycarbonyl-5,5-diphenyl-2,3,4-pentatrienoate, *in* D-70492

$C_{22}H_{20}O_5$
Alpinumisoflavone; Di-Me ether, *in* A-80050

$C_{22}H_{20}O_6$
Maximaisoflavone C, *in* T-80107
1-*O*-Methylglycyrol, *in* P-80186

$C_{22}H_{20}O_7$
2-(4-Allyl-2.6-dimethoxyphenoxy)-1-(4-hydroxy-3,5-dimethoxyphenyl)-1-propanol, *in* A-80046
Collybolide, *in* C-80147
Fernolin, F-80003
Isocollybolide, *in* C-80147
Pumilaisoflavone D, P-80194

$C_{22}H_{20}O_8$
ζ-Rhodomycinone, *in* R-70002
Thuriferic acid, T-70191

$C_{22}H_{20}O_9$
θ-Rhodomycinone, *in* R-70002
ε-Rhodomycinone, R-70002

$C_{22}H_{20}O_{10}$
ψ-Baptisin, *in* H-80203
Rothindin, *in* H-80203

$C_{22}H_{20}O_{11}$
Irilone-4′-glucoside, *in* D-80341
3′,4′,5,7-Tetrahydroxyisoflavone; 3′,4′-Methylene ether, 7-*O*-glucoside, *in* T-80109

$C_{22}H_{20}O_{13}$
Ellagic acid; 3,3′-Di-Me ether, 4-glucoside, *in* E-70007

$C_{22}H_{21}N$
1,3-Dibenzyl-1,3-dihydroisoindole, D-80077

$C_{22}H_{22}O_2$
Dodecahedranecarboxylic acid; Me ester, *in* D-80522

$C_{22}H_{22}O_4$
Paralycolin *A*, P-60009

$C_{22}H_{22}O_5$
Edulenane, *in* N-80023
Praecansone *B*, P-70113

$C_{22}H_{22}O_6$
Desmodin, *in* N-80023
2,3-Dibenzoylbutanedioic acid; Di-Et ester, *in* D-70083
Glycyrin, G-80031
Languiduline, L-80018
Neorautanin, *in* N-80022

$C_{22}H_{22}O_7$
1,8-Oxybis(ethyleneoxyethyleneoxy)-9,10-anthracenedione, O-80097

$C_{22}H_{22}O_8$
Peperomin A, P-80064
Picropodophyllin, *in* P-80165
▷ Podophyllotoxin, P-80165
Dalbergia Rotenolone, R-60014

$C_{22}H_{22}O_9$
Alternanthin, A-80053
Ononin, *in* H-80190

$C_{22}H_{22}O_{10}$
5,7-Dihydroxy-4′-methoxyflavone; 7-β-D-Galactoside, *in* D-70319
Echioidin, *in* T-80299
Glucoobtusifolin, *in* T-80322
8-*C*-Glucosyl-4′,5-dihydroxy-7-methoxyisoflavone, *in* G-80025
Prunitrin, *in* D-80335
Sissotrin, *in* D-80337
Sophojaponicin, *in* M-70001
Swertisin, S-80052
1,3,5,8-Tetrahydroxy-2-methylanthraquinone; 5-Me ether, 8-*O*-α-L-rhamnopyranoside, *in* T-60113
Tilianin, *in* D-70319
Trifolirhizin, *in* M-70001
3′,4′,7-Trihydroxyflavone; $O^{3'}$-Me, 7-glucoside, *in* T-80301
3′,4′,7-Trihydroxyisoflavone; 4′-Me ether, 7-*O*-glucoside, *in* T-80308

$C_{22}H_{22}O_{11}$
4-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2*H*-1-benzopyran-2-one; 7-Me ether, 5-*O*-β-D-galactopyranosyl, *in* D-70334
5-*O*-β-D-Glucopyranosyl-3′,4′-dihydroxy-7-methoxyneoflavone, *in* D-80356
8-*C*-Glucosyl-4′,5,7-trihydroxy-3′-methoxyisoflavone, *in* G-80024
Pratensein 7-*O*-glucoside, *in* T-80109
3′,4′,5,7-Tetrahydroxyisoflavone; 3′-Me ether, 7-*O*-glucoside, *in* T-80109

$C_{22}H_{23}NO$
Aminododecahedrane; *N*-Ac, *in* A-80071

$C_{22}H_{23}N_3O_9$
▷ Aluminon, *in* A-60318

$C_{22}H_{24}Br_2N_4O_6S_2$
N,N′-Bis[3-(3-bromo-4-hydroxyphenyl)-2-oximidopropionyl]cystamine, B-70130

$C_{22}H_{24}O_5$
Edulane, *in* N-80023
Quercetol *C*, Q-70003

$C_{22}H_{24}O_6$
Austrobailignan-7; Ac, *in* A-70271
Ramosissin, R-60001

$C_{22}H_{24}O_7$
7α-Acetoxybacchotricuneatin B, *in* B-80006
Actifolin, A-80036
Machilin *E*, *in* M-60003
Richardianidin 1, R-70006
Richardianidin 2, *in* R-70006

$C_{22}H_{24}O_8$
1-Acetoxypinoresinol, *in* H-60221
4,5;4′,5′-Bismethylenedioxypolemannone, *in* P-60166
Byakangelicin; *O*-Angeloyl, *in* B-80296
Skutchiolide B, S-70050

$C_{22}H_{24}O_9$
2,3-Dihydroononin, *in* D-80322
3,3′,4′,5,5′,7,8-Heptamethoxyflavone, *in* H-70021

$C_{22}H_{24}O_{10}$
Helichrysin, *in* H-80246
5-Hydroxy-3,3′,4′,5′,6,7,8-heptamethoxyflavone, *in* O-70018

$C_{22}H_{24}O_{11}$
Lanceolin/, *in* D-80372

$C_{22}H_{25}ClO_7$
Methyl 2,2′-di-*O*-methyleriodermate, *in* E-70032

$C_{22}H_{25}N_3$
Tris(methylphenylamino)methane, T-70324

$C_{22}H_{26}$
2,7-Di-*tert*-butyldicyclopenta[*a,e*]cyclooctene, D-70102
1,2,3,4,5,6,7,8-Octamethylanthracene, O-80018

$C_{22}H_{26}Br_2O_3$
4,21-Dibromo-3-ethyl-2,19-dioxabicyclo[16.3.1]docosa-6,9,18(22),21-tetraen-12-yn-20-one, *in* E-70042

$C_{22}H_{26}N_2$
2,5-Di-*tert*-butyl-2,5-dihydrobenzo[*e*]pyrrolo[3,4-*g*]isoindole, D-70103
2,7-Di-*tert*-butyl-2,7-dihydroisoindolo[5,4-*e*]isoindole, D-70104

$C_{22}H_{26}O_3$
Acetylimbricatolal, *in* H-70150
3-Ethyl-2,19-dioxabicyclo[16.3.1]docosa-3,6,9,18(22),21-pentaen-12-yn-20-one, E-70042

$C_{22}H_{26}O_4$
Dimethyldehydrodieugenol, *in* D-80023
21-Ethyl-2,6-epoxy-17-hydroxy-1-oxacyclohenicosa-2,5,14,18,20-pentaen-11-yn-4-one, E-60050

$C_{22}H_{26}O_5$
Aristoligone, *in* A-70251
Aristosynone, *in* A-70251
9-(1,3-Benzodioxol-5-yl)-1-(2,6-dihydroxyphenyl)-1-nonanone, *in* M-70007
Costatolide, C-80154
5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b′*]dipyran-2-one, *in* M-80001
Isodidymic acid, I-60098
Licarin *C*, L-60024
MAB 6, M-80001
Unanisoflavan, U-80002

$C_{22}H_{26}O_6$
Asebotin, *in* H-80244
Gelomulide E, *in* G-80008
Henricine, H-60017
Pachypostaudin B, P-80002

$C_{22}H_{26}O_7$
Glaucocalactone, G-80019
Heliopsolide; 8-Ac, *in* H-70007
Heliopsolide; 4-Epimer, 8-Ac, *in* H-70007
6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3*H*,9*H*-[1,2]-dioxolo[3′,4′:4,5]furo[2,3-*f*][1]benzopyran-3-one, H-80152
Laferin, L-60009
Praderin, P-70112
Sessein, S-60027
Teupyrenone, T-60184

$C_{22}H_{26}O_8$
Abbreviatin PB, A-60001
Albaspidin AP, *in* A-80043
3,6-Bis(3,4-dimethoxyphenyl)tetrahydro-1*H*,3*H*-furo[3,4-*c*]furan-1,4-diol, B-60156
Desaspidin AB, *in* D-80032
Euparotin acetate, *in* E-80090
Flavaspidic acids; Flavaspidic acid AB-*form*, *in* F-80011
Heliopsolide; 2α,3α-Epoxide, 8-Ac, *in* H-70007
Isopicropolin, I-60112
7-Oxodihydrogmelinol, O-60064

$C_{22}H_{26}O_9$
3′,4′,5,5′,6,7,8-Heptamethoxyflavanone, *in* H-80029
1-Hydroxysyringaresinol, *in* H-60221
Liscunditrin, *in* D-80006
Skutchiolide A, S-70049
1-(2,3,4,5-Tetramethoxyphenyl)-3-(2,4,5-trimethoxyphenyl)-1,3-propanedione, *in* T-70120

$C_{22}H_{26}O_{10}$
2′-*O*-Benzoylaucubin, *in* A-80186

$C_{22}H_{26}O_{11}$
Agnuside, *in* A-80186

$C_{22}H_{26}O_{13}$
Verproside, *in* C-70026

$C_{22}H_{28}$
Des-A-26,27-dinoroleana-5,7,9,11,13-pentaene, D-80033
Des-A-26,27-dinor-5,7,9,11,13-ursapentaene, D-80034
Nonacyclo[11.7.1.1^{2,18}.0^{3,16}.0^{4,13}.0^{5,10}.0^{6,14}.0^{7,11}.0^{15,20}]docosane, N-80067

$C_{22}H_{28}O_2$
Fervanol benzoate, *in* F-60007
Hydrallmanol A, H-80099

$C_{22}H_{28}O_3$
Fervanol *p*-hydroxybenzoate, *in* F-60007
Kurubasch aldehyde benzoate, *in* K-60014

$C_{22}H_{28}O_4$
1-(6-Hydroxy-2-methoxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone, *in* M-70007
Kurubashic acid benzoate, *in* K-60014
Verecynarmin *A*, V-60005

$C_{22}H_{28}O_5$
ent-14α-Acetoxy-7β-hydroxy-1,16-kauradiene-3,15-dione, *in* D-80324
ent-7β-Acetoxy-14α-hydroxy-1,16-kauradiene-3,15-dione, *in* D-80324
1α,10β-Epoxykurubaschic acid benzoate, *in* K-60014
1β,10α-Epoxykurubashic acid benzoate, *in* K-60014
Flabellata secoclerodane, F-70009
Ganschisandrine, G-80005
1-(6-Hydroxy-2-methoxyphenyl)-9-(3,4-methylenedioxyphenyl)-1-nonanone, *in* M-70007
19-*O-Acetyl*-1,2-*dehydrohautriwaic acid*, *in* H-70002

$C_{22}H_{28}O_6$
ent-2α-Acetoxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
ent-7β-Acetoxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80143
Articulin acetate, *in* A-60307
Chrysophyllin *B*, C-70175
8,9-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide; 9-Ac, 8-(2*R*,3*R*-epoxy-2-methylbutanoyl), *in* D-60323
Fragransin D_1, F-70040
Fragransin D_2, *in* F-70040

Fragransin D_3, *in* F-70040
Gelomulide B, G-80007
Gelomulide F, *in* G-80008
Homoheveadride, H-60089
Pachypophyllin, P-80001
Pachypostaudin A, *in* P-80002

$C_{22}H_{28}O_7$
ent-2α-Acetoxy-7β-hydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
ent-7β-Acetoxy-2α-hydroxy-3,13-clerodadiene-16,15:18,19-diolide, *in* H-80142
17-Acetoxythymifodioic acid, *in* T-60218
3-Acetylteumicropin, *in* T-60181
2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3-hydroxy-4,5-dimethoxyphenyl)-1-propanol, *in* A-80046
12-Epiteupolin II, *in* T-70159
Eupaserrin, *in* D-70302
Teupolin I, T-70159
Teupolin II, *in* T-70159

$C_{22}H_{28}O_8$
Citreoviridinol A_1, C-70181
Citreoviridinol A_2, *in* C-70181
5,5′-Dimethoxylariciresinol, *in* L-70019
Gracilin *B*, G-60034
Gracilin *C*, *in* G-60034
Hiyodorilactone D, H-80090
Hiyodorilactone E, *in* H-80090
Teuvincentin B, T-80167

$C_{22}H_{28}O_9$
8-Deacyltrichogoniolide; 8-*O*-Angeloyl, 9-Ac, *in* D-80007

$C_{22}H_{28}O_{10}$
8β,10β-Diacetoxy-1-*O*-methylhirsutinolide 13-*O*-acetate, *in* H-80089
8β-Propionyloxy-10β-hydroxyhirsutinolide 1,13-di-*O*-acetate, *in* H-80089

$C_{22}H_{29}ClO_7$
Solenolide E, S-70054

$C_{22}H_{30}$
Biadamantylideneethane, B-60075
Decamethylbiphenyl, D-80012

$C_{22}H_{30}O$
Uvarisesquiterpene B, U-80037

$C_{22}H_{30}O_3$
2-Hydroxy-6-(8,11,14-pentadecatrienyl)benzoic acid, *in* H-60205
Pseudopterosin *A*; Aglycone, *O*-Ac, *in* P-60187
Siccanin, S-60029
Siccanochromene *E*, S-60030

$C_{22}H_{30}O_4$
5-Epiilimaquinone, *in* I-80004
Ferolin, *in* G-60014
Ilimaquinone, I-80004
Metachromin A, M-70033
Metachromin C, M-80036

$C_{22}H_{30}O_5$
2α-Acetoxyhardwickiic acid, *in* H-70002
6β-Acetoxyhebemacrophyllide, *in* H-60010
ent-3α-Acetoxy-11α-hydroxy-16-kaurene-6,15-dione, *in* D-80325
3β-Acetoxy-19-hydroxy-13(16),14-spongiadien-2-one, *in* D-70345
7α-Acetoxyroyleanone, *in* D-80265
3β-Acetoxywedeliasecokaurenolide, *in* W-60004
Bretonin A, *in* D-80526
Brevifloralactone acetate, *in* B-70179
3,5-Di-*O*-methylsenecioodontol, *in* S-60022
Epoxyjaeschkeanadiol *p-hydroxybenzoate*, *in* J-70001
Feraginidin, *in* D-60004
Ferugin, *in* D-60005
Gelomulide A, *in* G-80008
Hautriwaic acid acetate, *in* H-70002
Isobretonin A, *in* D-80526
Lasianthin, L-60017
Pseudopterogorgia diterpenoid *B*, P-70128
5-*epi*-6β-*acetoxyhebemacrophyllide*, *in* H-60010

$C_{22}H_{30}O_6$
7α-Acetoxy-12,20-dihydroxy-8,12-abietadiene-11,14-dione, *in* R-60015
ent-3α-Acetoxy-1β,11α-dihydroxy-16-kaurene-6,15-dione, *in* T-80313
ent-12β-Acetoxy-7β,14α-dihydroxy-16-kaurene-3,15-dione, *in* T-80315
ent-1β-Acetoxy-7β,14α-dihydroxy-16-kaurene-3,15-dione, *in* T-80314
17-Acetoxygutiesolbriolide, *in* G-80045
17-Acetoxyisogutiesolbriolide, *in* I-80062
Isopregomisin, I-80077
Longikaurin *C*, *in* L-70035
Longikaurin *E*, *in* L-70035

$C_{22}H_{30}O_7$
6β-Acetoxypulchellin 4-*O*-angelate, *in* P-80189
Isomontanolide, *in* M-70154
Longikaurin *B*, *in* L-70035
Longikaurin *D*, *in* L-70035
Lophanthoidin C, *in* T-80084
Lophanthoidin E, *in* T-80084
Montanolide, M-70154

$C_{22}H_{30}O_8$
Maoecrystal I, M-80007

$C_{22}H_{32}N_2$
1,2-Diphenyl-1,2-ethanediamine; *N*-Tetra-Et, *in* D-70480

$C_{22}H_{32}O_2$
Dehydroabietinol acetate, *in* A-60007
Uvarisesquiterpene A, U-80036
Uvarisesquiterpene C, U-80038

$C_{22}H_{32}O_3$
Acetylsanadaol, *in* S-70008
3,4-Epoxy-13(15),16,18-sphenolobatrien-5-ol; Ac, *in* E-60031
2-Hydroxy-6-(8,11-pentadecadienyl)benzoic acid, H-60205

$C_{22}H_{32}O_4$
ent-18-Acetoxy-15-beyeren-19-oic acid, *in* H-60106
7β-Acetoxy-13(17),15-cleistanthadien-18-oic acid, *in* H-70115
19-Acetoxy-15,16-epoxy-13,17-spatadien-5α-ol, *in* E-60029
12β-Acetoxyisopimara-8(14),15-dien-18-oic acid, *in* S-80008
ent-1α-Acetoxy-16-kauren-19-oic acid, *in* H-80179
ent-3β-Acetoxy-15-kauren-17-oic acid, *in* H-60167
ent-3β-Acetoxy-16-kauren-18-oic acid, *in* H-80181
ent-6β-Acetoxy-7,12*E*,14-labdatrien-17-oic acid, *in* L-60004
Dictyodendrillolide, D-80149
Dilophus ether, D-80408
Iloprost, I-60003
Lagerstronolide, L-60010
5-Methoxy-3-(8,11,14)pentadecatrienyl)-1,2,4-benzenetriol, M-70049

$C_{22}H_{32}O_5$
ent-14*S*-Acetoxy-1β,7β-dihydroxy-16-kauren-15-one, *in* T-50476
ent-7β-Acetoxy-1β,14*S*-dihydroxy-16-kauren-15-one, *in* T-50476
ent-6β,17-Diacetoxy-14,15-bisnor-7,11*E*-labdadien-13-one, *in* D-60311
Grayanotoxin IX, *in* G-80040
Grayanotoxin X, *in* G-80040
7-Hydroxy-8(17),13-corymbidienolide, H-60110
4,10(14)-Oplopadiene-3,8,9-triol; 3-Ac, 8-angeloyl, *in* O-70042
4,10(14)-Oplopadiene-3,8,9-triol; 3-Ac, 9-angeloyl, *in* O-70042

$C_{22}H_{32}O_6$
5-Acetoxy-9α-angeloyloxy-8β-hydroxy-10(14)-oplopen-3-one, *in* T-70272
6α-Acetoxy-17β-hydroxy-15,17-oxido-16-spongianone, *in* D-60365
ent-3α-Acetoxy-2α,6β,11β-trihydroxy-16-kauren-15-one, *in* P-80047
Lophanthoidin D, *in* T-80084
Oleaxillaric acid, O-80042

$C_{22}H_{32}O_7$
Arguticinin, A-70250
Arguticinin; 4-Epimer, *in* A-70250

$C_{22}H_{32}O_8$
1,3,5,7-Adamantanetetracarboxylic acid; Tetra-Et ester, *in* A-80037

$C_{22}H_{32}O_{10}$
Rengyoside *C*, *in* R-80004

$C_{22}H_{33}BrO_4$
2α-Acetoxy-15-bromo-9(11)-parguerene-7α,16-diol, *in* B-80240

$C_{22}H_{33}BrO_5$
2α-Acetoxy-15-bromo-9(11)-parguerene-7α,16,19-triol, *in* B-80240

$C_{22}H_{34}N_8$
3,6,9,17,20,23,29,30-Octaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),11(30),12,14,25,27-hexaene, O-80003

$C_{22}H_{34}O_2$
ent-17-Acetoxy-9β*H*-isopimara-7,15-diene, *in* I-80075
19-Acetoxy-9,(11),15-pimaradiene, *in* P-80148

$C_{22}H_{34}O_3$
ent-3β-Acetoxy-15-kauren-17-ol, *in* K-60007
ent-6β-Acetoxy-7,12*E*,14-labdatrien-17-ol, *in* L-60004
Cladiellin, C-80137
10-Hydroxy-7,11,13,16,19-docosapentaenoic acid, H-70125
8-Hydroxy-5,9,11,14,17-eicosapentaenoic acid; Et ester, *in* H-70126
2-Hydroxy-6-(10-pentadecenyl)benzoic acid, *in* H-60205
2-Hydroxy-6-(8-pentadecenyl)benzoic acid, *in* H-60205

$C_{22}H_{34}O_4$
20-Acetoxy-2β,3α-dihydroxy-1(15),8(19)-trinervitadiene, *in* T-70299
2β-Acetoxy-8(17),13*E*-labdadien-15-oic acid, *in* H-70147
2β-Acetoxy-8(17),13*Z*-labdadien-15-oic acid, *in* H-70147
Dictyotriol *A*; 12-Ac, *in* D-70147
3β-Hydroxyisoagatholal; 3-Ac, *in* D-70310
Koanoadmantic acid, *in* H-70224
Maesanin, M-60004
1(15),8(19)-Trinervitadiene-2,3,9-triol; 9-Ac, *in* T-70298

$C_{22}H_{34}O_5$
6-Acetoxy-3,4-epoxy-12-hydroxy-7-dolabellen-16-al, *in* D-70541
4-Acetoxy-6-(4-hydroxy-4-methyl-2-cyclohexenyl)-2-(4-methyl-3-pentenyl)-2-heptenoic acid, A-60018
Cornudentanone, C-60167
3,4-Epoxy-13(15),16-sphenolobadiene-5,18-diol; 5-Ac, *in* E-60030
Stolonidiol acetate, *in* S-60055

$C_{22}H_{34}O_6$
7β-Acetoxy-8α,13*R*-epoxy-6β,9α-dihydroxy-14-labden-11-one, *in* E-80037
▷ Grayanotoxin IV, *in* G-80038
Grayanotoxin XVI, *in* G-80038

$C_{22}H_{34}O_7$
Coleonol, *in* E-70027
Coleonol B, *in* E-70027
Grayanotoxin XIII, *in* G-80038

$C_{22}H_{34}O_{11}$
Coleoside, *in* I-80078

$C_{22}H_{36}O_3$
ent-15-Acetoxy-7,13-labdadien-2α-ol, *in* L-80003
ent-15-Acetoxy-7,13-labdadien-2β-ol, *in* L-80004
19-Acetoxymanoyl oxide, *in* E-70023
Acetoxyodontoschismenol, *in* D-70541

Chromophycadiol monoacetate, *in* C-60148
8-Hydroxy-5,9,11,14,17-eicosapentaenoic acid; 17,18-Dihydro, Et ester, *in* H-70126
ent-8(17),13-Labdadiene-7α,15-diol; 7-Ac, *in* L-70006
Secotrinervitane, S-60019

$C_{22}H_{36}O_4$
6-Acetoxy-3,7-dolabelladiene-12,16-diol, *in* D-70541
19-Acetoxy-18-hydroxygeranylnerol, *in* B-80151
ent-3β-Acetoxy-16β,17-kauranediol, *in* K-60005
15-Acetoxy-7-labden-17-oic acid, *in* H-60168
Hamachilobene *E*, *in* H-70001
15-Hydroxy-7-labden-17-oic acid; Ac, *in* H-80183

$C_{22}H_{36}O_5$
Methyl 3,6-epidioxy-6-methoxy-4,16,18-eicosatrienoate, *in* E-60007

$C_{22}H_{36}O_7$
▷ Grayanotoxin I, *in* G-80039

$C_{22}H_{36}O_{16}$
Shanzhisin methyl ester gentiobioside, *in* S-60028

$C_{22}H_{36}S_6$
1,3,4,6-Tetrakis(*tert*-butylthio)thieno[3,4-*c*]thiophene, *in* T-70170

$C_{22}H_{39}NO_5$
Valilactone, V-70002

$C_{22}H_{40}N_4O_{14}P_2S_2$
Pantethine; 4,4′-Diphosphate, *in* P-80009

$C_{22}H_{40}O_4$
Ricinoleyl alcohol; Di-Ac, *in* O-60006

$C_{22}H_{41}NO_7$
Fumifungin, F-60082

$C_{22}H_{42}N_4O_8S_2$
Pantethine, P-80009

$C_{22}H_{42}O_4$
▷ Bis(2-ethylhexyl)adipate, B-80148

$C_{22}H_{46}$
2-Methylheneicosane, M-80091

$C_{23}H_{14}O$
7-Methoxyindeno[1,2,3-*cd*]pyrene, *in* I-60025
8-Methoxyindeno[1,2,3-*cd*]pyrene, *in* I-60026

$C_{23}H_{14}O_6$
1,8,11-Triptycenetricarboxylic acid, T-60398
1,8,14-Triptycenetricarboxylic acid, T-60399

$C_{23}H_{16}O$
4-(Diphenylmethylene)-1(4*H*)-naphthalenone, D-70487

$C_{23}H_{16}O_5$
Lophirone E, L-80040

$C_{23}H_{16}O_6$
2,2′-Methylenebis[8-hydroxy-3-methyl-1,4-naphthalenedione], M-70063

$C_{23}H_{17}N$
2*H*-Dibenz[*e,g*]isoindole; *N*-Benzyl, *in* D-70067

$C_{23}H_{18}$
4*b*,8*b*,13,14-Tetrahydrodiindeno[1,2-*a*:2′,1′-*b*]indene, T-70058

$C_{23}H_{18}O$
1-Oxa[2.2](2,7)naphthalenophane, O-80052

$C_{23}H_{18}O_2$
1,3-Diphenyl-1*H*-indene-2-carboxylic acid; Me ester, *in* D-60481

$C_{23}H_{18}O_7$
Antibiotic SS 43405*D*, A-70239
Rotenonone, *in* D-80026

$C_{23}H_{18}O_8$
Villosone, *in* S-80051

$C_{23}H_{20}N_2O$
Isoamarin; 1-Ac, *in* D-80263

$C_{23}H_{20}O_4$
1-Phenyl-1,2-propanediol; Dibenzoyl, *in* P-80121
1-Phenyl-1,3-propanediol; Dibenzoyl, *in* P-80122

$C_{23}H_{20}O_6$
Dehydrodeguelin, *in* D-80020
Dehydrorotenone, D-80026

$C_{23}H_{20}O_7$
Amorpholone, *in* D-80026
Dehydroamorphigenin, *in* A-80152
Dehydrotoxicarol, *in* T-80204
Ferrugone, F-80006
Ichthynone, I-80001
5-Methoxydurmillone, *in* D-80537
Villosol, *in* S-80051

$C_{23}H_{20}O_8$
Boesenboxide, B-70173
Desertorin *B*, *in* D-60022

$C_{23}H_{22}N_3O_3$
2,5-Dihydro-2,2,5,5-tetramethyl-3-[[[(2-phenyl-3*H*-indol-3-ylidene)amino]oxy]carbonyl]-1*H*-pyrrol-1-yloxy, D-60284

$C_{23}H_{22}O_5$
Isouvaretin, *in* U-80035
Uvaretin, U-80035

$C_{23}H_{22}O_6$
▷ Deguelin, D-80020
Gerontoxanthone A, G-80012
Gerontoxanthone B, G-80013
Myriconol, M-80204

$C_{23}H_{22}O_7$
▷ Amorphigenin, A-80152
Dehydrodalpanol, *in* D-80003
Sumatrol, S-80051
Tephrosin, T-80009
α-Toxicarol, T-80204

$C_{23}H_{22}O_8$
11-Hydroxytephrosin, *in* T-80009
Villosin, *in* S-80051

$C_{23}H_{22}O_{10}$
6″-*O*-Acetyldaidzin, *in* D-80323
Phrymarolin II, P-80140

$C_{23}H_{22}O_{11}$
6″-*O*-Acetylgenistin, *in* T-80309
Fujikinin, *in* T-80111

$C_{23}H_{23}NO_4$
1,4-Dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid; Dibenzyl ester, *in* D-80193

$C_{23}H_{24}O_5$
Demethoxyegonol 2-methylbutanoate, *in* E-70001
Praecansone *A*, *in* P-70113

$C_{23}H_{24}O_6$
BR-Xanthone *A*, B-70282
Gerontoxanthone C, G-80014

$C_{23}H_{24}O_7$
2-Acetoxyaristotetralone, *in* A-70253
Dalpanol, D-80003
Dihydroamorphigenin, *in* A-80152

$C_{23}H_{24}O_7S$
Floroselin, *in* K-70013
Isofloroselin, *in* K-70013

$C_{23}H_{24}O_8$
Amorphigenol, *in* A-80152
Loxodellonic acid, L-70039

$C_{23}H_{24}O_9$
Isovolubilin, I-80098
Wistin, *in* T-80310

$C_{23}H_{24}O_{10}$
Embigenin, *in* S-80052
4′,7,8-Trihydroxyisoflavone; 4′,8-Di-Me ether, 7-*O*-glucoside, *in* T-80311

$C_{23}H_{24}O_{11}$
Abrusin, A-80004
Eupalin, *in* P-80035
Flavoyadorinin *B*, *in* D-70291
Kakkalidone, *in* T-80112
4′,5,6,7-Tetrahydroxyisoflavone; 6,7-Di-Me ether, 4′-*O*-glucoside, *in* T-80112
Volubilinin, V-80012

$C_{23}H_{24}O_{12}$
Homotectoridin, *in* P-80045
Iristectorin A, *in* P-80043
Iristectorin B, *in* P-80043

$C_{23}H_{25}ClN_2O_9$
8-Methoxychlorotetracycline, M-70045

$C_{23}H_{25}ClN_2O_{10}$
4*a*-*Hydroxy*-8-*methoxychlorotetracycline*, *in* M-70045

$C_{23}H_{26}O_4$
6-Benzoyl-5,7-dihydroxy-2-methyl-2-(4-methyl-3-pentenyl)chroman, B-80056
2-Benzoyl-6-nerylphloroglucinol, *in* D-80460
3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzophenone, D-80460

$C_{23}H_{26}O_5$
5-Methoxy-2,2-dimethyl-6-(2-methyl-1-oxo-2-butenyl)-10-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-8-one, M-80042

$C_{23}H_{26}O_6$
Garvin *A*, G-60008
Teracrylshikonin, *in* S-70038

$C_{23}H_{26}O_7$
Neokadsuranin, N-70024
Stenosporonic acid, S-70072

$C_{23}H_{26}O_8$
1-Hydroxypinoresinol; 4″-Me ether, 1-Ac, *in* H-60221
Peperomin B, P-80065
Sikkimotoxin, S-60032

$C_{23}H_{26}O_{11}$
Lindleyin, L-80034
Macrophylloside *B*, *in* M-70004
Macrophylloside *C*, M-70004
Nyasicaside, *in* B-60155

$C_{23}H_{26}O_{13}$
β-Sorinin, *in* S-80039

$C_{23}H_{27}ClO_7$
3-Chlorostenosporic acid, *in* S-80044

$C_{23}H_{28}N_4O_7$
Biphenomycin *B*, *in* B-60114

$C_{23}H_{28}N_4O_8$
Biphenomycin *A*, B-60114

$C_{23}H_{28}O_3$
Citreomontanin, C-60149

$C_{23}H_{28}O_4$
2-Acetoxy-1,11-bis(3-furanyl)-4,8-dimethyl-3,6,8-undecatriene, *in* B-70143
Quercetol *B*, Q-70002

$C_{23}H_{28}O_5$
2α-Anisoyloxy-9-oxoisoanhydrooplopanone, *in* O-50045

$C_{23}H_{28}O_7$
Isosphaeric acid, I-60136
Palliferinin, *in* L-60014
Stenosporic acid, S-80044

$C_{23}H_{28}O_8$
Albaspidin AB, *in* A-80043
Albaspidin PP, *in* A-80043
Aspidin AB, *in* A-80180
Desaspidin PB, *in* D-80032
4,5-Dimethoxy-4′,5′-methylenedioxypolemannone, *in* P-60166
Flavaspidic acids; Flavaspidic acid PB-*form*, *in* F-80011
Methylenebisdesaspidinol BB, M-80077

$C_{23}H_{28}O_{10}$
Diffutin, *in* T-60103

$C_{23}H_{28}O_{13}$
Picroside II, *in* C-70026

$C_{23}H_{29}NO_6$
Fusarin *A*, F-60107

$C_{23}H_{29}NO_7$
Fusarin *D*, *in* F-60107

$C_{23}H_{30}O_4$
Fervanol vanillate, *in* F-60007
Guayulin *D*, *in* A-60299

$C_{23}H_{30}O_5$
3,5-Dihydroxy-19-oxo-14,20(22)-cardadienolide, D-80350
Ginamallene, G-80017
Kurubasch aldehyde vanillate, *in* K-60014

$C_{23}H_{30}O_7$
1,3-Bis[(2-methoxyethoxy)methoxy]-1,3-diphenyl-2-propanone, B-80154
Seco-4-hydroxylintetralin, S-70023

$C_{23}H_{30}O_8$
Acanthospermal *A*, A-60012
Gracilin *D*, *in* G-60034
Isorolandrolide; 13-Et ether, *in* I-80087

$C_{23}H_{32}O_2$
2,2′-Methylenebis[6-*tert*-butyl-4-methylphenol], M-80076

$C_{23}H_{32}O_3$
Avarol; 5′-Ac, *in* A-80189
Dictyoceratin, D-80148

$C_{23}H_{32}O_4$
8,11,13-Abietatrien-19-ol; 19-(Carboxyacetyl), *in* A-60007
6α-Anisoyloxy-1β,4β-epoxy-1β,10α-eudesmane, *in* E-80026
3-Eudesmene-1,6-diol; 6-Anisoyl, *in* E-80083
Metachromin B, M-70034
Methyl 11,12-dimethoxy-6,8,11,13-abietatrien-20-oate, *in* D-60305
Smenorthoquinone, S-80035

$C_{23}H_{32}O_5$
Chimganidin, *in* G-60014

$C_{23}H_{32}O_6$
16α-Acetoxy-2α,3β,12β-trihydroxy-4,7-pregnadien-20-one, *in* T-60124
Cannogeninic acid, C-80017
Epoxyjaeschkeanadiol vanillate, *in* J-70001
3,14,15-Trihydroxy-19-oxocard-20(22)-enolide, T-80330
8-Vanilloylshiromodiol, *in* S-70039

$C_{23}H_{32}O_7$
Lophanthoidin A, *in* T-80084

$C_{23}H_{32}O_9$
Absinthifolide, *in* H-60138

$C_{23}H_{34}$
Des-A-26-nor-5,7,9-lupatriene, D-80036

$C_{23}H_{34}O_4$
7,13-Corymbidienolide, C-60169
ent-17-Malonyloxy-9βH-isopimara-7,15-diene, *in* I-80075

$C_{23}H_{34}O_5$
Bryophollenone, B-80270
▷ Coroglaucigenin, C-60168
Dactylospongenone A, D-80002
Dactylospongenone B, *in* D-80002
Dactylospongenone C, *in* D-80002
Dactylospongenone D, *in* D-80002
Gracilin *A*, G-60033
4,10(14)-Oplopadiene-3,8,9-triol; 3-Ac, 9-(3-Methyl-2-pentenoyl), *in* O-70042

$C_{23}H_{34}O_6$
Coriolin *B*, *in* C-70199

$C_{23}H_{34}O_7$
Coriolin *C*, *in* C-70199

$C_{23}H_{36}O_5$
9,11-Dihydrogracilin *A*, *in* G-60033

$C_{23}H_{36}O_6$
Helogynic acid, H-70008

$C_{23}H_{38}O_4$
15-Hydroxy-7-labden-17-oic acid; 15-Ac, Me ester, *in* H-60168
12-Isoagathen-15-oic acid; 2,3-Dihydroxypropyl ester, *in* I-60085

$C_{23}H_{38}O_5$
Muamvatin, M-70156

$C_{23}H_{38}O_8$
Gaillardoside, *in* T-70284

$C_{23}H_{41}N_3O_2S$
Agelasidine C, A-80040

$C_{23}H_{45}N_5O_{12}$
Youlemycin, Y-70002

$C_{23}H_{46}$
3-Tricosene, T-80234
9-Tricosene, T-60259

$C_{23}H_{46}O_3$
2-Hydroxytricosanoic acid, H-80259

$C_{24}H_{12}$
[4]Phenylene, P-60089

$C_{24}H_{12}N_4O_4$
25,26,27,28-Tetraazapentacyclo[19.3.1.1^{3,7}.1^{9,13}.1^{15,19}]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-2,8,14,20-tetrone, T-70010

$C_{24}H_{12}O_2$
1,1′-Biacenaphthylidene-2,2′-dione, B-80067

$C_{24}H_{12}S_3$
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tris[1]benzothiophene, B-60052
Benzo[1,2-*b*:3,4-*b*′:6,5-*b*″]tris[1]benzothiophene, B-60053

$C_{24}H_{14}$
Benz[5,6]indeno[2,1-*a*]phenalene, B-70025
1,1′-Bibiphenylene, B-60080
2,2′-Bibiphenylene, B-60081
Dibenz[*e*,*k*]acephenanthrylene, D-70066
Indeno[1,2,3-*hi*]chrysene, I-70010

$C_{24}H_{14}O_2$
Indeno[1,2,3-*cd*]pyren-1-ol; Ac, *in* I-60022
Indeno[1,2,3-*cd*]pyren-2-ol; Ac, *in* I-60023
Indeno[1,2,3-*cd*]pyren-6-ol; Ac, *in* I-60024

$C_{24}H_{14}O_6$
6,7-Dihydroxy-1,12-perylenedione; Di-Ac, *in* D-80354

$C_{24}H_{15}N_3$
Diindolo[3,2-*a*:3′,2′-*c*]carbazole, D-60384

$C_{24}H_{16}$
Cyclodeca[1,2,3-*de*:6,7,8-*d*′*e*′]dinaphthalene, C-60187
Cycloocta[1,2-*b*:5,6-*b*′]dinaphthalene, C-60216
1,2:9,10-Dibenzo[2.2]metaparacyclophane, D-70071
1,2:7,8-Dibenzo[2.2]paracyclophane, D-70072
1-(Diphenylmethylene)-1*H*-cyclopropa[*b*]naphthalene, D-70485

$C_{24}H_{16}O_2$
5,6,10,11,16,17,21,22-Octadehydro-7,9,18,20-tetrahydrodibenzo[*e*,*n*][1,10]dioxacyclo-octadecin, O-70006

$C_{24}H_{16}O_6$
Lophirone D, L-80039

$C_{24}H_{17}N$
10,11-Dihydro-5*H*-diindeno[1,2-*b*;2′,1′-*d*]pyrrole; *N*-Ph, *in* D-80182

$C_{24}H_{17}N_3$
2,3′:2′,3″-Ter-1*H*-indole, T-60011

$C_{24}H_{18}$
1,2,9,10,17,18-Hexadehydro[2.2.2]paracyclophane, H-60038

$C_{24}H_{18}N_6O_{12}$
Benzo[1,2-*b*:3,4-*b*′:5,6-*b*″]tripyrazine-2,3,6,7,10,11-tetracarboxylic acid; Hexa-Me ester, *in* B-60051

$C_{24}H_{18}O_{10}$
Eriocephaloside, *in* H-70133

$C_{24}H_{20}$
[2.2](2,6)Azulenophane, A-60355
7-(Diphenylmethylene)-2,3,5,6-tetramethylenebicyclo[2.2.1]heptane, D-70488
2,5,8,11-Tetramethylperylene, T-70140
3,4,9,10-Tetramethylperylene, T-70141

$C_{24}H_{20}N_2$
4(5)-Vinylimidazole; 1-Triphenylmethyl, *in* V-70012

$C_{24}H_{20}O$
3,4,4-Triphenyl-2-cyclohexen-1-one, T-60379
3,5,5-Triphenyl-2-cyclohexen-1-one, T-60380
4,5,5-Triphenyl-2-cyclohexen-1-one, T-60381

$C_{24}H_{20}O_5$
8-Dihydrocinnamoyl-5,7-dihydroxy-4-phenyl-2*H*-benzopyran-2-one, D-60210

$C_{24}H_{20}O_8$
Kielcorin *B*, K-60012

$C_{24}H_{20}O_9$
Subalatin, S-80048

$C_{24}H_{20}S_2$
7*H*,9*H*,16*H*,18*H*-Dinaphtho[1,8-*cd*:1′,8′-*ij*][1,7]dithiacyclododecin, D-70448
2,3-Naphthalenedithiol; Di-*S*-benzyl, *in* N-70004

$C_{24}H_{22}O_7$
Lepidissipyrone, L-80023

$C_{24}H_{22}O_8$
Desertorin *C*, *in* D-60022
Villinol, *in* S-80051

$C_{24}H_{22}O_{13}$
Genistein 7-*O*-glucoside 6″-malonate, *in* T-80309

$C_{24}H_{23}N$
5,5,9,9-Tetramethyl-5*H*,9*H*-quino[3,2,1-*de*]acridine, T-70143

$C_{24}H_{24}O_{11}$
5-*O*-(6-Acetyl-β-D-galactopyranosyl)-3′,4′-dihydroxy-7-methoxyneoflavone, *in* D-80356
Phrymarolin I, *in* P-80140

$C_{24}H_{24}O_{12}$
Dalpatin, *in* P-80042
3′,4′,5,6,7-Pentahydroxyisoflavone; 5,6-Di-Me, 3′,4′-methylenedioxy ether, 7-*O*-β-D-glucopyranoside, *in* P-80043
Platycarpanetin 7-*O*-glucoside, *in* P-80045

$C_{24}H_{25}NO_8$
Antibiotic Sch 38519, A-60287

$C_{24}H_{26}$
1,3,6-Triphenylhexane, T-60386

$C_{24}H_{26}O_4$
15-Cinnamoyloxyisoalloalantolactone, *in* I-80047
(E)-ω-Oxoferprenin, *in* F-70003
Isoalloalantolactone; 15-Cinnamoyloxy (*Z*-), *in* I-80047

$C_{24}H_{26}O_6$
Egonol 2-methylbutanoate, *in* E-70001

$C_{24}H_{26}O_7$
(+)-Anomalin, *in* K-70013
(−)-Anomalin, *in* K-70013
Anomalin, *in* K-70013
Calipteryxin, *in* K-70013
Khellactone; Bis(3-methyl-3-butenoyl), *in* K-70013
Khellactone; Di-*O*-(3-Methyl-2-butenoyl), *in* K-70013
Khellactone; O^9-(3-Methyl-2-butenoyl), O^{10}-angeloyl, *in* K-70013
Peuformosin, *in* K-70013

$C_{24}H_{26}O_8$
Drummondin C, D-80532
Khellactone; O^9-Angeloyl, O^{10}-(2,3-Epoxy-2-methylbutanoyl), *in* K-70013

$C_{24}H_{26}O_9$
Khellactone; Di-*O*-(2,3-Epoxy-2-methylbutanoyl), *in* K-70013

$C_{24}H_{26}O_{10}$
Sophoraside *A*, *in* P-70137

$C_{24}H_{26}O_{11}$
3′,4′,6,7-Tetrahydroxyisoflavone; 3′,4′,6-Tri-Me ether, 7-*O*-β-D-glucopyranoside, *in* T-80111
4′,5,7,8-Tetrahydroxyisoflavone; 4′,5,8-Tri-Me ether, 7-*O*-β-D-glucoside, *in* T-80113
4′,5,6,7-Tetrahydroxyisoflavone; 4′,5,6-Tri-Me ether, 7-*O*-glucoside, *in* T-80112

$C_{24}H_{26}O_{13}$
Iridin, *in* H-80071
Jacein, *in* H-80067
Sudachiin A, *in* T-80341
4′,5,7-Trihydroxy-3′,6,8-trimethoxyflavone; 7-*O*-β-D-Glucopyranoside, *in* T-80341

$C_{24}H_{27}ClN_2O_9$
8-Methoxy-*N-methylchlorotetracycline*, *in* M-70045

$C_{24}H_{27}N_2O_8P$
Thymidine 5′-phosphate; Dibenzyl ester, *in* T-80196

$C_{24}H_{27}N_3$
Hexahydro-1,3,5-triazine; 1,3,5-Tribenzyl, *in* H-60060

$C_{24}H_{27}N_3O_6$
Physarochrome *A*, P-60150

$C_{24}H_{28}$
2-(9-Decenyl)phenanthrene, D-80019

$C_{24}H_{28}O_2$
3,7-Di-*tert*-butyl-9,10-dimethyl-2,6-anthraquinone, D-60113

$C_{24}H_{28}O_3$
Ferprenin, F-70003
4-Geranyl-3,4′,5-trihydroxystilbene, G-70008

$C_{24}H_{28}O_4$
2α-Cinnamoyloxy-9-oxoisoanhydrooplopanone, *in* O-50045
6,6′;7,3*a*′-Diligustilide, D-70363
(E)-ω-Hydroxyferprenin, *in* F-70003
(E)-ω-Oxoferulenol, *in* F-80007
Riligustilide, R-60009
Ternatin, T-70008
(Z)-ω-Hydroxyferprenin, *in* F-70003

$C_{24}H_{28}O_5$
Aphyllocladone, A-70242

$C_{24}H_{28}O_7$
Garcinone *D*, G-70004
Khellactone; *O*-Angeloyl, *O*-3-methylbutanoyl, *in* K-70013
Khellactone; *O*-Angeloyl, *O*-2-methylpropanoyl, *in* K-70013
Khellactone; O^9-(3-Methylbutanoyl), O^{10}-angeloyl, *in* K-70013

$C_{24}H_{28}O_{11}$
Decumbeside *A*, *in* G-60002
Decumbeside *B*, *in* G-60002
Globularicisin, *in* C-70026
Globularin, *in* C-70026
Macrophylloside *A*, *in* M-70004

$C_{24}H_{28}O_{12}$
Scutellarioside II, *in* C-70026

$C_{24}H_{28}O_{14}$
α-Sorinin, *in* S-80039

$C_{24}H_{29}ClO_8$
Ptilosarcenone, P-70136
Ptilosarcenone, *in* P-60193

$C_{24}H_{29}ClO_9$
11-Hydroxyptilosarcenone, *in* P-60193
Teuvincentin A, T-80166

$C_{24}H_{30}$
1,1′-Diphenylbicyclohexyl, D-70475
1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydro-1,4:5,8:9,12-triethanotriphenylene, D-80525

$C_{24}H_{30}O_3$
Ferulenol, F-80007
Guayulin *C*, *in* A-60299
9α-Hydroxygymnomitryl cinnamate, *in* G-70035

$C_{24}H_{30}O_4$
Assafoetidin, A-70265
6β-Cinnamoyloxy-1α-hydroxy-5,10-bisepi-4-eudesmen-3-one, *in* H-80101
3,8-Dihydro-6,6′;7,3′*a*-diliguetilide, D-60223
(E)-ω-Hydroxyferulenol, *in* F-80007
Gummosin, *in* P-80166
(Z)-ω-Hydroxyferulenol, *in* F-80007

$C_{24}H_{30}O_5$
Asacoumarin A, A-80173
Asacoumarin B, A-80174
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *in* M-80001
5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, *in* M-80001
Kopeolone, *in* K-80012
Praealtin B, *in* P-80172
Praealtin C, *in* P-80172

$C_{24}H_{30}O_6$
Magnoshinin, M-60007

$C_{24}H_{30}O_7$
Khellactone; Bis(3-methylbutanoyl), *in* K-70013

$C_{24}H_{30}O_8$
Aemulin BB, A-80039
Albaspidin PB, *in* A-80043
Desaspidin BB, *in* D-80032
Flavaspidic acid, *in* F-80011
Montanin *C*, *in* T-70159
Peperomin C, P-80066
Saroaspidin *A*, S-70012

$C_{24}H_{30}O_9$
Auropolin, A-60319
Montanin *G*, M-70153
Teumicropodin, T-60182

$C_{24}H_{30}O_{10}$
Dichotosinin, *in* T-60103

$C_{24}H_{30}O_{11}$
Globularidin, *in* C-70026

$C_{24}H_{30}O_{12}$
Syringopicroside *B*, *in* S-60067

$C_{24}H_{30}O_{13}$
Secologanol; 7-(2,5-Dihydroxybenzoyl), *in* S-80016

$C_{24}H_{31}ClO_8$
12-Ptilosarcenol, P-60193

$C_{24}H_{31}ClO_{10}$
Solenolide C, S-70053

$C_{24}H_{32}$
Pentacyclo[12.2.2.2^{2,5}.2^{6,9}.2^{10,13}]tetracosa-1,5,9,13-tetraene, P-60029

$C_{24}H_{32}O_3$
Antheliolide A, A-70213
6α-Cinnamoyloxy-1β,4β-epoxy-1β,10α-eudesmane, *in* E-80026
3-Eudesmene-1,6-diol; 1-Cinnamoyl, *in* E-80083
3-Eudesmene-1,6-diol; 6-Cinnamoyl, *in* E-80083

$C_{24}H_{32}O_4$
Antheliolide B, *in* A-70213
Karatavicinol, K-80004

$C_{24}H_{32}O_5$
6β-Cinnamoyloxy-3β-hydroperoxy-5,10-bisepi-4-eudesmen-1α-ol, *in* H-80101
6β-Cinnamoyloxy-4β-hydroperoxy-5,10-bisepi-2-eudesmen-1α-ol, *in* H-80102
6β-Cinnamoyloxy-3β-hydroperoxy-1α-hydroxy-5,10-bisepi-4(15)-eudesmene, *in* E-80084
Kopeolin, K-80012

$C_{24}H_{32}O_6$
Okilactomycin, O-70030
Spongiadiol; Di-Ac, *in* D-70345
Verrucosidin, V-60006

$C_{24}H_{32}O_7$
16-Acetoxy-12-*O*-acetylhorminone, *in* D-80265
9β-Acetoxy-1α-benzoyloxy-4β,6β-dihydroxydihydro-β-agarofuran, *in* T-80090
Furcellataepoxylactone, F-70052
Isoschizandrin, I-70101
Palliferin, *in* L-60014

$C_{24}H_{32}O_8$
Acetylisomontanolide, *in* M-70154
Exidonin, E-80093
Ganervosin A, G-80004
Hydroxyniranthin, H-70187
Jodrellin A, J-80013
Longikaurin *F*, *in* L-70035
Lophanthoidin B, *in* T-80084
Maeocrystal *J*, *in* M-80007
Nirphyllin, N-80032
4,4′,5,5′-Tetramethoxypolemannone, *in* P-60166

$C_{24}H_{33}ClO_9$
13-Deacetyl-11(9)-havannachlorohydrin, *in* H-70004
Solenolide B, *in* S-70052

$C_{24}H_{34}N_2O_3$
1,4,10-Trioxa-7,13-diazacyclopentadecane; 4,10-Dibenzyl, *in* T-60376

$C_{24}H_{34}O_4$
▷ Bufalin, B-70289

$C_{24}H_{34}O_5$
12-(Acetyloxy)-10-[(acetyloxy)methylene]-6-methyl-2-(4-methyl-3-pentenyl)-2,6,11-dodecatrienal, A-70049
Carotdiol veratrate, *in* D-80004
Dilophus enone, D-80407

$C_{24}H_{34}O_6$
ent-3β,19-Diacetoxy-15-kauren-17-oic acid, *in* D-60341
Paniculadiol; Di-Ac, *in* P-80007

$C_{24}H_{34}O_7$
ent-3α,6β-Diacetoxy-2α,11β-dihydroxy-16-kauren-15-one, *in* P-80047
ent-1β,3α-Diacetoxy-11α,15α-dihydroxy-16-kauren-6-one, *in* K-80008
6α,17α-Diacetoxy-15,17-oxido-16-spongianone, *in* D-60365
Lophanthoidin F, *in* T-80084

$C_{24}H_{34}O_8$
Solenolide F, S-70055
Teucretol, T-60179

$C_{24}H_{35}BrO_5$
2α,16-Diacetoxy-15-bromo-9(11)-pargueren-7α-ol, *in* B-80240

$C_{24}H_{36}$
Heptacyclo[19.3.0.0^{1,5}.0^{5,9}.0^{9,13}.0^{13,17}.0^{17,21}]tetracosane, H-80017

$C_{24}H_{36}O_4$
ent-6β,17-Diacetoxy-7,12*E*,14-labdatriene, *in* L-60004
Soulattrone *A*, S-70057

$C_{24}H_{36}O_5$
ent-6β,17-Diacetoxy-7,11*E*,14-labdatrien-13ξ-ol, *in* L-60005
1(15),8(19)-Trinervitadiene-2,3,9-triol; 2,3-Di-Ac, *in* T-70298

$C_{24}H_{36}O_6$
6α-Butanoyloxy-17β-hydroxy-15,17-oxido-16-spongianone, *in* D-60365
Hamachilobene *B*, *in* H-70001
1(15),8(19)-Trinervitadiene-2β,3α,9β,20-tetrol 9,20-diacetate, *in* T-70296

$C_{24}H_{36}O_7$
ent-1β,3α-Diacetoxy-16-kaurene-6β,11α,15α-triol, *in* K-80008

$C_{24}H_{36}O_8$
Lapidolin, *in* L-60015

$C_{24}H_{38}$
Des-A-5(10),12-oleanadiene, D-80037
Des-A-5(10),12-ursadiene, D-80039

$C_{24}H_{38}O_3$
Leiopathic acid; Et ester, *in* H-70125

$C_{24}H_{38}O_4$
Trifarin, T-70236
Trunculin *A*, T-60408

$C_{24}H_{38}O_5$
6,16-Diacetoxy-3,7-dolabelladien-12-ol, *in* D-70541
ent-3β,17-Diacetoxy-16β-kauranol, *in* K-60005
Trunculin *B*, T-60409

$C_{24}H_{38}O_6$
7β,15-Diacetoxy-8-labden-17-oic acid, *in* D-80330
Hamachilobene *A*, H-70001
Hamachilobene *C*, *in* H-70001
Hamachilobene *D*, *in* H-70001

$C_{24}H_{38}O_8$
Rhodojaponin IV, *in* G-80039

$C_{24}H_{40}$
Des-A-lup-9-ene, D-80035
Des-A-lup-5(10)-ene, *in* D-80035

$C_{24}H_{40}O_2$
3-Hydroxy-22,23,24,25,26,27-hexanor-20-dammaranone, H-60151

$C_{24}H_{40}O_4$
15,17-Diacetoxy-7-labdene, *in* L-80012

$C_{24}H_{40}O_5$
3,11,15-Trihydroxycholanic acid, T-60317
3,15,18-Trihydroxycholanic acid, T-60318

$C_{24}H_{42}$
10β*H*-Des-A-lupane, *in* D-80035
1,3,5-Trihexylbenzene, T-70247

$C_{24}H_{42}O_4$
Bisdihydrotrifarin, *in* T-70236

$C_{24}H_{43}NO_7$
2-Amino-1,3,4-hexadecanetriol; *O,N,N,N*-Tetra-Ac, *in* A-80079

$C_{24}H_{44}O_4$
7,11,15-Trimethyl-3-methylene-1,2-hexadecanediol; Di-Ac, *in* T-60368

$C_{24}H_{46}$
12-Tetracosyne, T-70018
1-Tetracosyne, T-70017

$C_{24}H_{46}N_4O_8S_2$
Homopantethine, *in* H-60090

$C_{24}H_{47}NO_{11}S$
N-[15-(β-D-Glucopyranosyloxy)-8-hydroxypalmitoyl]taurine, G-70019

$C_{24}H_{50}$
3-Methyltricosane, M-80185

$C_{25}H_{14}O$
Benzo[*a*]naphtho[2,1-*d*]fluoren-9-one, B-80027
Benzo[*b*]naphtho[2,1-*d*]fluoren-9-one, B-80028

$C_{25}H_{16}$
Spirobi[9*H*-fluorene], S-60040

$C_{25}H_{16}O_2$
Benz[*a*]anthracen-10-ol; O-Benzoyl, *in* B-80011

$C_{25}H_{20}N_2$
Triphenylphenylazomethane, T-70312

$C_{25}H_{21}N$
3,5-Dimethyl-2,4,6-triphenylpyridine, D-80478

$C_{25}H_{22}$
[2](1,5)Naphthaleno[2](2,7)(1,6-methano[10]annuleno)phane, N-70005

$C_{25}H_{22}O_6$
Cudraflavone *A*, C-70205
2-Hydroxymethyl-1,3-propanediol; Tribenzoyl, *in* H-80212

$C_{25}H_{22}O_7$
Artobiloxanthone, A-80172
Cycloartobiloxanthone, C-80173
5′-Hydroxycudraflavone *A*, *in* C-70205

$C_{25}H_{22}O_8$
Galtamycinone, *in* G-70003

$C_{25}H_{22}O_9$
Hypericorin, H-70234
Silandrin, S-70042
Silyhermin, S-70045
Silymonin, *in* S-70044

$C_{25}H_{22}O_{10}$
Isosilybin, I-70102
Isosilychristin, I-70103
Silydianin, S-70044

$C_{25}H_{22}O_{12}$
Daphnorin, *in* D-70006

$C_{25}H_{24}$
Bicyclo[18.4.1]pentacosa-1,3,5,7,9,11,13,15,17,19,21,23-dodecaene, B-80089
5,5*a*,6,6*a*,7,12,12*a*,13,13*a*,14-Decahydro-5,14:6,13:7,12-trimethanopentacene, D-60010

$C_{25}H_{24}O_2S$
3-[(Triphenylmethyl)thio]cyclopentanecarboxylic acid, *in* M-60021

$C_{25}H_{24}O_5$
Euchrenone A_1, E-70056
Isochandalone, I-80052
Isomammeigin, I-70069

$C_{25}H_{24}O_6$
Cudraisoflavone *A*, C-70206
Isoauriculatin, *in* P-80015

$C_{25}H_{24}O_7$
Laserpitinol, *in* L-60016

$C_{25}H_{24}O_{12}$
3,4-Di-*O*-caffeoylquinic acid, D-70110
7-Hydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonylglucoside), *in* H-80190

$C_{25}H_{24}O_{13}$
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-D-glucoside), *in* D-80337

$C_{25}H_{26}O_4$
Abyssinone III, A-80008
Erybraedin D, E-80051

$C_{25}H_{26}O_5$
Cajaflavanone, C-60004
Euchrenone A_2, E-70057
Honyucitrin, H-70092
Sigmoidin E, S-80032
4′,5,7-Trihydroxy-3′,6-bis(3-methyl-2-butenyl)isoflavone, T-80290

$C_{25}H_{26}O_6$
Cajanone, C-80009
Fremontone, F-80081
2′-Hydroxyisolupalbigenin, H-80177
Kuwanol C, K-80014
Lupinisoflavone G, L-80044
Lupinisol A, L-80047
Lupinisolone A, L-80049
Orotinin, O-60044

$C_{25}H_{26}O_7$
Garvalone *B*, G-60005
Lupinisoflavone H, *in* L-80044
Lupinisoflavone I, L-80045
Lupinisoflavone J, L-80046
Lupinisol B, *in* L-80047
Lupinisol C, L-80048
Lupinisolone B, L-80050
Lupinisolone C, L-80051

$C_{25}H_{26}O_8$
Rhynchosperin *C*, *in* R-60007

$C_{25}H_{26}O_9$
Glomellonic acid, *in* G-70018

$C_{25}H_{26}O_{10}$
Fridamycin *A*, F-70043
Fridamycin *B*, *in* F-70043

$C_{25}H_{28}O_4$
Abyssinone IV, A-80009
Abyssinone VI, A-80010
1-[2,4-Dihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-3-(4-hydroxyphenyl)-2-propen-1-one, D-60310
Erythrabyssin II, E-80053
Isolinderatone, *in* L-70030
Linderachalcone, L-80032
Linderatone, L-70030

$C_{25}H_{28}O_5$
Abyssinone V, *in* A-80009
Ammothamnidin, A-70204
10′,11′-Dehydrocyclolycoserone, *in* C-70229
8,9-Dehydroircinin 1, *in* I-60083
Kuwanol D, K-80015
Lehmannin, L-70027
Lespedazaflavone *B*, L-60021
Lonchocarpol *A*, L-60030
Rhinacanthin B, *in* R-80005
Senegalensein, S-70034

$C_{25}H_{28}O_6$
Lonchocarpol *C*, L-60031
Lonchocarpol *D*, L-60032

$C_{25}H_{28}O_7$
Lonchocarpol *E*, L-60033

$C_{25}H_{28}O_8$
Drummondin B, D-80531
Glomelliferonic acid, G-70018

$C_{25}H_{28}O_{10}$
Egonol glucoside, *in* E-70001

$C_{25}H_{28}O_{13}$
2′,4′,5,5′,6,7-Hexahydroxyisoflavone; 2′,4′,5′,6-Tetra-Me ether, 7-*O*-glucoside, *in* H-80069
Isocaviudin, *in* H-80070

$C_{25}H_{28}O_{14}$
Gentioside, *in* T-80347
1-Hydroxy-3-methoxy-7-primeverosyloxyxanthone, *in* T-80347
7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone, *in* T-80347

$C_{25}H_{30}Cl_2O_6$
Napyradiomycin A_2, N-70016

$C_{25}H_{30}N_8O_9$
7-Hydro-8-methylpteroylglutamylglutamic acid, H-60096

$C_{25}H_{30}O_3$
2′-Epiisotriptiliocoumarin, *in* I-80096
Isotriptiliocoumarin, I-80096
Triptiliocoumarin, T-80363

$C_{25}H_{30}O_4$
4-Hydroxy-5-methyl-3-(3,8,11-trimethyl-8-oxo-2,6,10-dodecatrienyl)-2*H*-1-benzopyran-2-one, H-70183
5′-Hydroxytriptiliocoumarin, *in* T-80363
8-Hydroxytriptiliocoumarin, *in* T-80363
Linderatin, L-50048
Nassauvirevolutin *B*, *in* N-80014

$C_{25}H_{30}O_5$
Cyclolycoserone, C-70229
Cyclolycoserone; 3′-Epimer, *in* C-70229
1-(2,4-Dihydroxyphenyl)-3-[3,4-dihydroxy-2-(3,7-dimethyl-2,6-octadienyl)phenyl]-1-propanone, D-80357
1′-Epilycoserone, *in* L-70045

6′,7′-Epoxy-5′α-hydroxytriptiliocoumarin, *in* T-80363
Gypothamniol, G-70037
4-Hydroxy-3-(9-hydroxy-8-oxofarnesyl)-5-methylcoumarin, *in* H-70183
Ircinin 1, I-60083
Ircinin 2, *in* I-60083
Isolycoserone, I-70068
Lycoserone, L-70045

$C_{25}H_{30}O_6$
1-[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,5,6-tetrahydroxyphenyl]-3-(4-hydroxyphenyl)-1-propanone,9CI, D-80459
10′-Hydroxycyclolycoserone, *in* C-70229
10′-Hydroxy-1′-epilycoserone, *in* L-70045
10′-Hydroxyisolycoserone, *in* I-70068

$C_{25}H_{30}O_7$
Lonchocarpol *B*, *in* L-60030

$C_{25}H_{30}O_{13}$
Picroside III, *in* C-70026

$C_{25}H_{31}^{\oplus}$
2,3,4,5,6,7,8,10,11,12,13,?-Dodecahydro-1,4:5,8:10,13-triethano-1*H*-tribenzo[*a*,*c*,*e*]cycloheptenylium(1+), D-80524

$C_{25}H_{31}ClO_7$
3-Chloroperlatolic acid, *in* P-80070

$C_{25}H_{31}Cl_3O_6$
Napyradiomycin B_4, N-70017

$C_{25}H_{31}Cl_6Sb$
2,3,4,5,6,7,8,10,11,12,13,?-Dodecahydro-1,4:5,8:10,13-triethano-1*H*-tribenzo[*a*,*c*,*e*]cycloheptenylium(1+); Hexafluoroantimonate, *in* D-80524

$C_{25}H_{31}N_3O_5$
1-[*N*-[3-(Benzoylamino)-2-hydroxy-4-phenylbutyl]alanyl]proline, B-60056

$C_{25}H_{32}O_4$
Ircinianin, I-60081
Ircinic acid, I-60082
Nassauvirevolutin A, N-80014
Nassauvirevolutin C, N-80015

$C_{25}H_{32}O_5$
5-Oxo-8(10)*E*-variabilin, *in* V-80002
5-Oxovariabilin, *in* V-80002
Variabilin/; 5-Oxo, $\Delta^{8(10)}$(*E*-), Δ^{13}-isomer, *in* V-80002

$C_{25}H_{32}O_6$
3-*O*-Angeloylsenecioodontol, *in* S-60022

$C_{25}H_{32}O_7$
Ichangensin, I-70001
Perlatolic acid, P-80070

$C_{25}H_{32}O_8$
Albaspidin BB, *in* A-80043
Aspidin BB, *in* A-80180
Clausenolide, C-80140
Saroaspidin *B*, S-70013

$C_{25}H_{32}O_{10}$
Tinosporaside, T-80198

$C_{25}H_{32}O_{12}$
Isoligustroside, I-60104

$C_{25}H_{32}O_{13}$
Oleuroside, O-70038
Syringopicroside *C*, *in* S-60067

$C_{25}H_{33}ClO_8$
Punaglandin 3, P-70143

$C_{25}H_{33}ClO_{11}$
Tetragonolide isobutyrate, *in* T-80053

$C_{25}H_{33}NO$
Aurachin *D*, A-60315

$C_{25}H_{33}NO_2$
Aurachin *B*, A-60314
Aurachin *C*, *in* A-60315

$C_{25}H_{33}NO_3$
Aurachin *A*, A-60313

$C_{25}H_{34}O_3$
3-Anhydro-6-epiophiobolin *A*, *in* O-70040
Apo-12′-violaxanthal, *in* P-60065

$C_{25}H_{34}O_4$
Fasciculatin, F-70001
Isofasciculatin, *in* F-70001
Variabilin/, V-80002
Variabilin/; 20*E*-Isomer, *in* V-80002
Variabilin/; Δ^{13}-Isomer (*Z*-), *in* V-80002

$C_{25}H_{34}O_5$
5-Hydroxyvariabilin, *in* V-80002

$C_{25}H_{34}O_7$
Glycinoeclepin *A*, G-70022

$C_{25}H_{35}ClO_8$
Punaglandin 4, *in* P-70143

$C_{25}H_{36}O_3$
8-Deoxyophiobolin J, *in* O-70041
Persicaxanthin, P-60065

$C_{25}H_{36}O_4$
Elasclepic acid, *in* B-80064
6-Epiophiobolin *A*, *in* O-70040
5-[13-(3-Furanyl)-2,6,10-trimethyl-6,8-tridecadienyl]-4-hydroxy-3-methyl-2(5*H*)-furanone, F-70050
24-Methyl-25-nor-12,24-dioxo-16-scalaren-22-oic acid, M-60105
▷ Ophiobolin *A*, O-70040
Ophiobolin J, O-70041

$C_{25}H_{36}O_5$
8-Hydroxyvariabilin, *in* V-80002
Monoalide, M-70152
Salvileucolidone, S-70005
Thorectolide, T-70189

$C_{25}H_{36}O_6$
Pseudopterosin *A*, P-60187
Triflorestevione, T-70237

$C_{25}H_{36}O_7$
Bacchabolivic acid; Xylopyranoside, *in* B-80004

$C_{25}H_{36}O_{12}$
Kickxioside, K-70014

$C_{25}H_{37}NO_3$
Smenospongorine, *in* S-80036

$C_{25}H_{38}O_3$
Elasclepiol, *in* B-80064
Luffariellolide, L-70040
Palauolide, P-60001

$C_{25}H_{38}O_4$
Aglajne 2, A-70073
Spongiolactone, S-60047

$C_{25}H_{38}O_4S$
Suvanine, S-70085

$C_{25}H_{38}O_5$
Pallinin, *in* C-60021

$C_{25}H_{38}O_6$
Clibadic acid, C-70186
Desoxodehydrolaserpitin, *in* D-70009
Secopseudopterosin *A*, S-70026
Tingitanol, *in* D-70009

$C_{25}H_{38}O_7$
Isolaserpitin, *in* D-70009
Laserpitine, L-60016
Methyl 15α,17β-diacetoxy-15,16-dideoxy-15,17-oxido-16-spongianoate, *in* T-60038

$C_{25}H_{40}O_3$
4,6,8,10,12,14,16-Heptamethyl-6,8,11-octadecatriene-3,5,13-trione, H-70022
3-Octadecene-1,2-diol; 1-Benzoyl, *in* O-60005

$C_{25}H_{40}O_6$
2α-Angeloyloxy-8β,20-epoxy-14-labdene-3α,7α,13*R*-triol, *in* E-80036
Salvisyriacolide, S-60004

$C_{25}H_{40}O_8$
ent-3,13-Clerodadiene-15,16,17-triol; 17-*O*-β-Xylopyranoside, *in* C-80141

$C_{25}H_{42}O_4$
6β-Isovaleroyloxy-8,13*E*-labdadiene-7α,15-diol, *in* L-60003
Sclareol; 6α-Angeloyloxy, *in* S-70018

$C_{25}H_{45}FeN_6O_8$
Ferrioxamine *B*, F-60003

$C_{26}H_6N_8$
11,11,12,12,13,13,14,14-Octacyano-1,4:5,8-anthradiquinotetramethane, O-70002

$C_{26}H_{10}N_2O_6S_2$
Dibenzo[*b*,*m*]triphenodithiazine-5,7,9,14,16,18(8*H*,17*H*)-tetrone, D-70082

$C_{26}H_{14}$
Benz[*def*]indeno[1,2,3-*hi*]chrysene, B-70024
Benz[*def*]indeno[1,2,3-*qr*]chrysene, B-70023
Benzo[*h*]naphtho[2′,3′:3,4]cyclobuta[1,2-*a*]biphenylene, B-80025
Bisbenzo[3,4]cyclobuta[1,2-*c*;1′,2′-*g*]phenanthrene, B-60143
Fluoreno[9,1,2,3-*cdef*]chrysene, F-70017
Fluoreno[3,2,1,9-*defg*]chrysene, F-70016
Hexa[7]circulene, H-80037
Naphtho[1,2,3,4-*ghi*]perylene, N-60009

$C_{26}H_{14}O_2$
6,15-Hexacenedione, H-60033

$C_{26}H_{16}$
9,9′-Bifluorenylidene, B-60104

$C_{26}H_{18}$
1,3-Di-(1-naphthyl)benzene, D-60454
1,3-Di(2-naphthyl)benzene, D-60455

$C_{26}H_{18}N_2$
9,9′-Biacridylidene, B-70090
2,11-Diphenyldipyrrolo[1,2-*a*:2′,1′-*c*]quinoxaline, D-70479

$C_{26}H_{18}N_6$
7,11:20,24-Dinitrilodibenzo[*b*,*m*][1,4,12,15]tetraazacyclodocosine, D-60456

$C_{26}H_{18}O_9$
5,6,8,13-Tetrahydro-1,7,9,11-tetrahydroxy-8,13-dioxo-3-(2-oxopropyl)benzo[*a*]naphthacene-2-carboxylic acid, T-70095

$C_{26}H_{20}$
Tribenzotritwistatriene, T-70210

$C_{26}H_{20}N_2$
Diphenylketazine, D-80512

$C_{26}H_{20}N_4S$
N-2-Benzothiazolyl-*N*,*N*′,*N*″-triphenylguanidine, B-70057

$C_{26}H_{20}O$
Tetraphenylethanone, T-60167

$C_{26}H_{20}O_4$
Tetraphenoxyethene, T-80157

$C_{26}H_{20}O_6$
1,8,11-Triptycenetricarboxylic acid; Tri-Me ester, *in* T-60398
1,8,14-Triptycenetricarboxylic acid; Tri-Me ester, *in* T-60399

$C_{26}H_{20}O_7$
Imbricatonol, I-70003

$C_{26}H_{20}O_{10}$
Salvianolic acid *C*, *in* S-70003

$C_{26}H_{20}S_3$
3,3,5,5-Tetraphenyl-1,2,4-trithiolane, T-70153

$C_{26}H_{22}N_2O$
1,1,1′,1′-Tetraphenyldimethylamine; *N*-Nitroso, *in* T-70150

$C_{26}H_{22}O_4$
1,2-Di-2-naphthalenyl-1,2-ethanediol; Di-Ac, *in* D-80479

$C_{26}H_{22}O_6$
Stypandrol, S-50130

$C_{26}H_{22}Se_2$
Bis(diphenylmethyl) diselenide, B-70141

$C_{26}H_{23}N$
1,1,1′,1′-Tetraphenyldimethylamine, T-70150

$C_{26}H_{24}$
Tricyclo[18.4.1.1^{8,13}]hexacosa-2,4,6,8,10,12,14,16,18,20,22,24-dodecaene, T-60263
Tricyclo[18.4.1.1.^{8,13}]hexacosa-2,4,6,8,10,12,14,16,18,20,22,24-dodecaene, T-80241

$C_{26}H_{24}N_6$
1,14,29,30,31,32-Hexaazahexacyclo[12.7.7.1^{3,7}.1^{8,12}.1^{16,20}.1^{23,27}]dotriaconta-3,5,7(32),8,10,12(31),16,18,20(30),23,25,27(29)-dodecaene, H-70030

$C_{26}H_{24}O_2$
[2.2][2.2]Paracyclophane-12,15-quinone, P-60008
[2.2][2.2]Paracyclophane-5,8-quinone, P-60007

$C_{26}H_{24}O_{10}$
Peltigerin, P-70016

$C_{26}H_{24}O_{15}$
4,6-Di-*O*-*galloylarbutin*, *in* A-70248

$C_{26}H_{25}N_3O_{11}$
Tunichrome B-1, T-70336

$C_{26}H_{26}$
[2.2]Paracyclo(4,8)[2.2]metaparacyclophane, P-60005

$C_{26}H_{26}O_2S$
4-[(Triphenylmethyl)thio]cyclohexane-carboxylic acid, *in* M-60020

$C_{26}H_{26}O_7$
Cajaisoflavone, C-80008

$C_{26}H_{26}O_9$
Dukunolide *A*, D-60522

$C_{26}H_{26}O_{10}$
Dukunolide *B*, *in* D-60522

$C_{26}H_{26}O_{12}$
7-Hydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonylglucoside), Me ester, *in* H-80190

$C_{26}H_{26}O_{13}$
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-D-glucoside), Me ester, *in* D-80337

$C_{26}H_{26}O_{18}$
Amritoside, *in* E-70007

$C_{26}H_{28}O_6$
2′-*O*-Methylcajanone, *in* C-80009
Orotinichalcone, O-60043
Orotinin; 5-Me ether, *in* O-60044
3,4,7,8-Tetrahydro-11-(2-hydroxy-4-methoxyphenyl)-2,2,6,6-tetramethyl-2*H*,6*H*,12*H*-benzo[1,2-*b*;3,4-*b*′;5,6-*b*″]tripyran-12-one, T-80067
3,4,7,8-Tetrahydro-11-(2-hydroxy-4-methoxyphenyl)-2,2,6,6-tetramethyl-2*H*,6*H*,12*H*-benzo[1,2-*b*;3,4-*b*′;5,6-*b*″]tripyran-12-one; 2′-Deoxy, 3′-hydroxy, *in* T-80067

$C_{26}H_{28}O_8$
Acidissimin, A-80034
Dukunolide *D*, D-60523

$C_{26}H_{28}O_9$
Dukunolide *E*, *in* D-60523
Dukunolide *F*, *in* D-60523
Ephemeroside, *in* E-60006

$C_{26}H_{28}O_{10}$
Jasmolactone C, J-80007

$C_{26}H_{28}O_{13}$
Ambonin, *in* D-80323
Neobanin, *in* D-80323

$C_{26}H_{28}O_{14}$
Ambocin, *in* T-80309
Neobacin, *in* T-80309
Neocorymboside, N-70021
1,2,7-Trihydroxy-6-methylanthraquinone; O^2-β-Primeveroside, *in* T-70268

$C_{26}H_{28}O_{19}$
Luteolic acid; Diglucoside, *in* L-80052

$C_{26}H_{29}NO_9$
Antibiotic R 20Y7, A-70230

$C_{26}H_{29}N_3O_2$
Crystal violet lactone, C-70202

$C_{26}H_{29}N_3O_{11}S_2$
O^6-[(3-Carbamoyl-2*H*-azirine-2-ylidene)amino]-1,2-*O*-isopropylidene-3,5-di-*O*-tosyl-α-D-glucofuranoside, C-70014

$C_{26}H_{29}O_{14}^{\oplus}$
Pelargonidin 3-sambubioside, *in* T-80093

$C_{26}H_{30}Cl_2N_2O_5$
Antibiotic SF 2415A_3, A-70234

$C_{26}H_{30}N_2O_5$
Antibiotic SF 2415A_2, A-70233

$C_{26}H_{30}N_6$
5,6,11,12-Tetrahydro-5,6,11,12,13,20-hexamethyl-5*a*,11*a*-(imino[1,2]benzenimino)quinoxalino[2,3-*b*]quinoxaline, T-80064

$C_{26}H_{30}O_4$
2′,6′-Dihydroxy-4′-methoxy-3′-(1-p-menthen-3-yl)chalcone, D-80338
Erycristin, E-70034
Grenoblone, G-70029
Methyllinderatone, *in* L-70030

$C_{26}H_{30}O_5$
(E)-ω-Acetoxyferprenin, *in* F-70003
4-Hydroxygrenoblone, *in* G-70029
(Z)-ω-Acetoxyferprenin, *in* F-70003

$C_{26}H_{30}O_6$
7-Deacetoxy-7-oxogedunin, *in* G-70006
2,3-Dibenzoylbutanedioic acid; Dibutyl ester, *in* D-70083
Lespedezaflavanone *A*, L-60022

$C_{26}H_{30}O_8$
Butyrylmallotochromene, B-80295
Drummondin A, D-80530
Dysoxylin, D-60525
Isobutyrylmallotochromene, I-80050

$C_{26}H_{30}O_{10}$
Graucin *A*, G-60036
Isolimonexic acid, *in* L-80031
Limonexic acid, L-80031

$C_{26}H_{30}O_{11}$
Rutaevinexic acid, R-70014

$C_{26}H_{30}O_{13}$
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one; 2′-[*O*-Rhamnosyl(1→4)xyloside], *in* H-80246
Liquiraside, *in* D-80367

$C_{26}H_{31}ClN_2O_5$
Antibiotic SF 2415A_1, A-70232

$C_{26}H_{32}Cl_2O_5$
Antibiotic SF 2415B_3, A-70237

$C_{26}H_{32}O_4$
Methyllinderatin, *in* L-50048
Nimbocinol, *in* A-70281

$C_{26}H_{32}O_5$
Antibiotic SF 2415B_2, A-70236
7-Deacetyl-17β-hydroxyazadiradione, *in* A-70281
(E)-ω-Acetoxyferulenol, *in* F-80007
Helihumulone, H-80006
Licoricidin, L-60025
Polyanthin, P-80166
Polyanthinin, *in* P-80166
(Z)-ω-Acetoxyferulenol, *in* F-80007

$C_{26}H_{32}O_6$
4′-(3,6-Dimethyl-2-heptenyloxy-5-hydroxy-3′,7-dimethoxyflavanone, *in* T-70105
7-*O*-(3-Hydroxy-7-drimen-11-yl)isofraxidin; 3-Ketone, *in* H-80158

$C_{26}H_{32}O_7$
3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-4-hydroxy-5,6-dimethyl-2*H*-pyran-2-one, A-80021

$C_{26}H_{32}O_8$
Longirabdosin, L-70036

$C_{26}H_{32}O_9$
Clausenarin, C-80139

$C_{26}H_{32}O_{10}$
Hiyodorilactone F, *in* H-80090
Teuvincentin C, T-80168

$C_{26}H_{32}O_{11}$
Columbinyl glucoside, *in* C-60160

$C_{26}H_{32}O_{12}$
1-Hydroxypinoresinol; 1-*O*-β-D-Glucopyranoside, *in* H-60221
1-Hydroxypinoresinol; 4′-*O*-β-D-Glucopyranoside, *in* H-60221
Isojateorinyl glucoside, *in* C-60160
Jateorinyl glucoside, *in* C-60160

$C_{26}H_{32}O_{13}$
Decumbeside *C*, D-60017
Decumbeside *D*, *in* D-60017
Haenkeanoside, H-80001
Isohaenkeanoside, *in* H-80001

$C_{26}H_{32}O_{14}$
Mulberroside *A*, *in* D-70335

$C_{26}H_{33}ClO_5$
Antibiotic SF 2415B_1, A-70235

$C_{26}H_{33}ClO_8$
Ptilosarcenone; 2-De-Ac, 2-butanoyl, *in* P-70136

$C_{26}H_{33}ClO_9$
Junceellolide B, J-80016
12-Ptilosarcenol; 12-Ac, *in* P-60193

$C_{26}H_{33}ClO_{10}$
Junceellolide A, J-80015
Junceellolide C, *in* J-80016

$C_{26}H_{33}ClO_{11}$
Solenolide D, *in* S-70053

$C_{26}H_{34}O_6$
7-*O*-(3-Hydroxy-7-drimen-11-yl)isofraxidin, H-80158
Nimolicinoic acid, N-60022

$C_{26}H_{34}O_7$
Salannic acid, S-80002

$C_{26}H_{34}O_8$
Agrimophol, A-60066
6β,9β-Diacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran, *in* T-80090
Saroaspidin *C*, S-70014
2,11,12-Trihydroxy-6,7-seco-8,11,13-abietatriene-6,7-dial 11,6-hemiacetal; Tri-Ac(6α-), *in* T-80339

$C_{26}H_{34}O_9$
Adenanthin, A-70065
Bryophyllin B, B-80272
Deoxyhavannahine, *in* H-60008
ent-1β,7α,11α-Triacetoxy-3α-hydroxy-16-kaurene-6,15-dione, *in* T-60109

$C_{26}H_{34}O_{10}$
9α,14-Diacetoxy-1α-benzoyloxy-4β,6β,8β-trihydroxydihydro-β-agarofuran, *in* E-60018
Eumaitenin, E-60071
Havannahine, H-60008
Rhynchospermoside *A*, R-60008
Rhynchospermoside *B*, *in* R-60008

$C_{26}H_{34}O_{11}$
Methyl 12,17;15,16-diepoxy-6-hydroxy-19-nor-17-oxo-4,13(16),14-clerodatrien-18-oate; *O*-β-D-Glucopyranoside, *in* M-80068

$C_{26}H_{35}ClO_{10}$
11(19)-Havannachlorohydrin, H-70004
7(18)-Havannachlorohydrin, H-70003

$C_{26}H_{35}ClO_{11}$
Tetragonolide 2-methylbutyrate, *in* T-80053

$C_{26}H_{36}$
[14.0]Paracyclophane, P-70008

$C_{26}H_{36}O_7$
14-Acetoxy-2-butanoyloxy-5,8(17)-briaradien-18,7-olide, *in* E-70012
9-Deacetoxyxenicin, *in* X-70004

$C_{26}H_{36}O_8$
Jodrellin B, *in* J-80013
ent-2α,3α,6β-Triacetoxy-7α,11β-dihydroxy-16-kauren-15-one, *in* P-80047

$C_{26}H_{36}O_9$
Caesalpin *F*, C-60002
Weisiensin A, *in* P-80048

$C_{26}H_{36}O_{10}$
Melianolone, M-60015

$C_{26}H_{38}O_4$
Aglajne 3, A-70074
12-Hydroxy-24-methyl-24-oxo-16-scalarene-22,25-dial, H-60191

$C_{26}H_{38}O_5$
Chinensin II, C-60036
12α-Hydroxy-24-methyl-24,25-dioxo-14-scalaren-22-oic acid, *in* H-60191

$C_{26}H_{38}O_6$
1-Acetoxy-7-acetoxymethyl-3-acetoxymethylene-11,15-dimethyl-1,6,10,14-hexadecatetraene, A-70020

$C_{26}H_{38}O_7$
17α-Acetoxy-6α-butanoyloxy-15,17-oxido-16-spongianone, *in* D-60365
Virescenoside *E*, *in* I-70081

$C_{26}H_{39}NO_3$
Smenospongianine, *in* S-80036

$C_{26}H_{40}N_4$
5,8,14,17-Tetrakis(dimethylamino)[3.3]paracyclophene, T-70126

$C_{26}H_{40}O_4$
16-Hydroxy-24-methyl-12,24-dioxo-25-scalaranal, H-80200

$C_{26}H_{40}O_5$
Episalviaethiopisolide, *in* S-80004
Salviaethiopisolide, S-80004

$C_{26}H_{40}O_7$
Virescenoside *L*, *in* I-70081

$C_{26}H_{40}O_8$
Virescenoside *G*, *in* I-70077

$C_{26}H_{40}O_9$
Phloganthoside, *in* P-70099

$C_{26}H_{40}O_{11}$
Rabdoside 1, *in* M-80008

$C_{26}H_{40}O_{12}$
Rabdoside 2, *in* M-80008

$C_{26}H_{40}O_{13}$
Jasmesosidic acid, J-80004

$C_{26}H_{40}O_{14}$
6′-*O*-Apiosylebuloside, *in* E-60001
9″-Hydroxyjasmesosidic acid, *in* J-80004

$C_{26}H_{42}N_6$
1,3,5,7-Tetrakis(diethylamino)pyrrolo[3,4-*f*]isoindole, T-70125

$C_{26}H_{42}O_2$
24-Nor-7,22-cholestadiene-3,6-diol, N-80078

$C_{26}H_{42}O_8$
Virescenoside *A*, *in* I-70081

$C_{26}H_{42}O_9$
Grayanoside *B*, *in* G-80041
Grayanoside C, *in* G-80041

$C_{26}H_{44}O_4N_4$
1,3,5,7-Adamantanetetraacetic acid; Tetrakis(dimethylamide), *in* A-70064

$C_{26}H_{46}O_6$
Sclareol; 13-(6′-Deoxy-α-L-idopyranoside), *in* S-70018

$C_{26}H_{48}O_3$
Ficulinic acid A, F-60011

$C_{26}H_{48}O_5$
5,6-Dihydro-6-(2,4,6-trihydroxyheneicosyl)-2*H*-pyran-2-one, D-70276

$C_{26}H_{48}O_6$
5,6-Dihydro-6-(2,4,6,10-tetrahydroxyheneicosyl)-2*H*-pyran-2-one, *in* D-70276

$C_{26}H_{50}O_2$
Aparjitin, A-60291

$C_{26}H_{50}O_4$
Bis(2-ethylhexyl) decanedioate, B-80149

$C_{26}H_{52}O$
Hexacosanal, H-80038

$C_{26}H_{54}$
3-Methylpentacosane, M-80131

$C_{26}H_{54}O$
5-Methyl-5-pentacosanol, M-80132

$C_{27}H_{14}$
Indeno[2,1,7,6-*ghij*]naphtho[2,1,8,7-*nopq*]pleiadene, I-80011

$C_{27}H_{20}$
1,2,3-Triphenyl-1*H*-indene, T-60387

$C_{27}H_{20}Cl_{15}N$
Tetraethylammonium tris(pentachlorophenyl)methylide, *in* T-60405

$C_{27}H_{20}O_7$
Mulberrofuran *R*, M-60149

$C_{27}H_{22}O$
1,1,3,3-Tetraphenyl-2-propanone, T-60168

$C_{27}H_{22}S_2$
4,4,5,5-Tetraphenyl-1,3-dithiolane, T-60166

$C_{27}H_{24}$
1,2,3-Trimethyl-4,5,6-triphenylbenzene, T-70291
1,2,4-Trimethyl-3,5,6-triphenylbenzene, T-70292
1,3,5-Trimethyl-2,4,6-triphenylbenzene, T-70293

$C_{27}H_{24}O_7$
Larreantin, L-70020

$C_{27}H_{26}O_4S_2$
Lappaphen a, L-70018
Lappaphen b, *in* L-70018

$C_{27}H_{26}O_7$
Euchrenone b_3, E-70059

$C_{27}H_{26}O_{11}$
Cleistanthoside *B*, *in* D-60493
Viscutin 1, *in* T-60103

$C_{27}H_{28}O_7$
Pumilaisoflavone *A*, P-70140
Pumilaisoflavone *B*, P-70141

$C_{27}H_{28}O_{11}$
Tremulacin, *in* S-70002

$C_{27}H_{28}O_{13}$
3-*O*-*Caffeoyl*-4-O-sinapoylquinic acid, *in* C-70005

$C_{27}H_{30}O_6$
Cyclotriveratrylene, C-70254
Glabrescione B, *in* T-80109

$C_{27}H_{30}O_7$
Pumilaisoflavone C, P-80193

$C_{27}H_{30}O_8$
5-Dehydrooriciopsin, *in* O-70045
Lacinolide A, L-80015

$C_{27}H_{30}O_{12}$
4′,7-Dihydroxyisoflavone; 4′,7-Di-*O*-rhamnoside, *in* D-80323

$C_{27}H_{30}O_{13}$
4′,7-Dihydroxyisoflavone; 7-*O*-(Rhamnosylglucoside), *in* D-80323
Podophyllotoxin; 4′-*O*-De-Me, 1-*O*-β-D-glucoside, *in* P-80165

$C_{27}H_{30}O_{14}$
4′,7-Dihydroxyisoflavone; 4′,7-Di-*O*-β-D-glucopyranosyl, *in* D-80323
Lanceolarin, *in* D-80337
Sophorabioside, *in* T-80309
Sphaerobioside, *in* T-80309

$C_{27}H_{30}O_{15}$
Orobol rhamnosylglucoside, *in* T-80109
Palasitrin, *in* S-70082
Paniculatin, P-80008
4′,5,6,7-Tetrahydroxyisoflavone; 7-*O*-Rhamnosylglucside, *in* T-80112
4′,5,7-Trihydroxyisoflavone; 4′,7-Di-*O*-glucoside, *in* T-80309
4′,5,7-Trihydroxyisoflavone; 7-*O*-Glucosylglucoside, *in* T-80309

$C_{27}H_{30}O_{16}$
Isoorientin; 4′-Glucoside, *in* I-80068
Lutonarin, *in* I-80068
3′,4′,5,7-Tetrahydroxy-6-*C*-sophorosylflavone, *in* I-80068

$C_{27}H_{30}O_{18}$
6,8-Di-*C*-glucosyl-3′,4′,5,7-tetrahydroxyisoflavone, D-80168

$C_{27}H_{31}O_{15}^{\oplus}$
Pelargonidin 3-sophoroside, *in* T-80093
Pelargonin, *in* T-80093

$C_{27}H_{32}O_6$
Scutellone *F*, S-70020

$C_{27}H_{32}O_7$
7-(2,4-Dimethoxyphenyl)-3,4-dihydro-5-hydroxy-10-(3-hydroxy-3-methylbutyl)-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, D-80415
7-(3,4-Dimethoxyphenyl)-3,4-dihydro-5-hydroxy-10-(3-hydroxy-3-methylbutyl)-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,6-*b*′]dipyran-6-one, D-80416
Garvalone *A*, G-60004

$C_{27}H_{32}O_8$
Oriciopsin, O-70045

$C_{27}H_{32}O_9$
Pedonin, P-60014
Trijugin *B*, T-60352

$C_{27}H_{32}O_{10}$
Baccharinoid B25, B-60004
Eumaitenol, E-60072

$C_{27}H_{32}O_{13}$
Aloinoside B, *in* B-80010
Aloinoside B, *in* B-80010
Cascaroside C, *in* B-80010
Cascaroside D, *in* B-80010
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one; 4′-*O*-α-L-Rhamnopyranoside, *in* D-80367
Rhamnoisoliquiritin, *in* D-80367

$C_{27}H_{32}O_{14}$
Cascaroside A, *in* B-80010
Cascaroside B, *in* B-80010
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one; 4′-*O*-Glucosylglucoside, *in* D-80367
Pyrenoside, P-80206

$C_{27}H_{32}O_{15}$
Isobutrin, *in* D-80362

$C_{27}H_{32}O_{16}$
3′,4′,5,7-Tetrahydroxyflavanone; 3′,5-Di-*O*-β-D-Glucoside, *in* T-70105

$C_{27}H_{33}N_3O_5$
Andrimide, A-60272

$C_{27}H_{34}O_4$
5-Oxocystofuranoquinol, *in* C-70260
5-Oxoisocystofuranoquinol, *in* C-70260
Yezoquinolide, Y-60003

$C_{27}H_{34}O_5$
Licoricidin; 7-Me ether, *in* L-60025
Scopadulcic acid *B*, *in* S-60015

$C_{27}H_{34}O_6$
Scopadulcic acid *A*, S-60015

$C_{27}H_{34}O_7$
6-Deoxyswietenolide, *in* S-80054
Scuterivulactone *D*, *in* T-70103

$C_{27}H_{34}O_8$
3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one, *in* A-80021
Swietenolide, S-80054

$C_{27}H_{34}O_9$
Isocyclocalamin, I-60096

$C_{27}H_{34}O_{11}$
Arctiin, *in* A-70249
Phillyrin, *in* P-60141

$C_{27}H_{34}O_{13}$
O-Methylhaenkeanoside, *in* H-80001
O-Methylisohaenkeanoside, *in* H-80001

$C_{27}H_{35}ClO_9$
12-Ptilosarcenol; 12-Propanoyl, *in* P-60193

$C_{27}H_{36}O_3$
Cystofuranoquinol, C-70260

$C_{27}H_{36}O_4$
16-(2,5-Dihydroxy-3-methylphenyl)-2,6,10,19-tetramethyl-2,6,10,14-hexadecatetraene-4,12-dione, *in* H-70225
5-Hydroxycystofuranoquinol, *in* C-70260

$C_{27}H_{36}O_7$
12α-Hydroxy-4,4,14α-trimethyl-3,7,11,15-tetraoxo-5α-chol-8-en-24-oic acid, *in* L-60037
Hyperlatolic acid, H-60236
Isohyperlatolic acid, I-60101
Planaic acid, P-80158

$C_{27}H_{36}O_8$
Clausenolide; 1-Et ether, *in* C-80140

$C_{27}H_{36}O_9$
4,14-Diacetoxy-2-propanoyloxy-5,8(17)-briaradien-18,7-olide, *in* E-70012

$C_{27}H_{36}O_{14}$
Sylvestroside III, S-70088
Sylvestroside IV, S-70089

$C_{27}H_{37}ClO_{10}$
Punaglandin 1, P-70142

$C_{27}H_{38}O$
10′-Apo-β-caroten-10′-ol, A-70246

$C_{27}H_{38}O_2$
Galloxanthin, G-70002
Sargaquinone, S-60010

$C_{27}H_{38}O_4$
8′,9′-Dihydroxysargaquinone, *in* S-60010
Sargahydroquinoic acid, S-60009

$C_{27}H_{38}O_5$
Amentadione, A-60086
Amentaepoxide, A-60087
Amentol, A-60088
Bifurcarenone, B-80093

$C_{27}H_{38}O_6$
Monoalide 25-acetate, *in* M-70152
Thorectolide 25-acetate, *in* T-70189

$C_{27}H_{38}O_7$
3β,12β-Dihydroxy-4,4,14α-trimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, *in* L-60037
3β-Hydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, *in* L-60036
Pseudopterosin *B*, *in* P-60187
Pseudopterosin *C*, *in* P-60187
Pseudopterosin *D*, *in* P-60187

$C_{27}H_{38}O_8$
3β,12β-Dihydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, *in* L-60036

$C_{27}H_{38}O_9$
Tirucalicine, T-80199

$C_{27}H_{38}O_{13}$
Macrocliniside *B*, *in* Z-60001

$C_{27}H_{38}O_{14}$
Laciniatoside V, L-80014

$C_{27}H_{39}ClO_{10}$
Punaglandin 2, *in* P-70142

$C_{27}H_{40}O_3$
2-(5-Hydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-6-methyl-1,2-benzenediol, H-70225

$C_{27}H_{40}O_4$
2-(5,16-Dihydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-6-methyl-1,4-benzenediol, *in* H-70225
Furoscalarol, F-70057

$C_{27}H_{40}O_5$
Chinensin I, C-60035

$C_{27}H_{40}O_7$
Lucidenic acid *H*, L-60036
Secopseudopterosin *B*, *in* S-70026
Secopseudopterosin *C*, *in* S-70026
Secopseudopterosin *D*, *in* S-70026

$C_{27}H_{40}O_9$
Methyl 6α,15α,17β-triacetoxy-15,16-dideoxy-15,17-oxido-16-spongianoate, *in* T-60038

$C_{27}H_{42}O$
Papakusterol, P-60004

$C_{27}H_{42}O_2$
Cholesta-7,9(11),22-triene-3,6-diol, C-80126

$C_{27}H_{42}O_3$
3,6-Dihydroxy-7,25-cholestadien-24-one, D-80302
25(27)-Spirosten-3-ol, S-70065
5-Spirosten-3-ol, S-60045

$C_{27}H_{42}O_4$
Deacetoxybrachycarpone, *in* B-60195
6-Hydroxy-3-spirostanone, H-70219
Nuatigenin, N-60062
5-Spirostene-3,25-diol, S-60044

$C_{27}H_{42}O_5$
24-Acetoxy-12-deacetyl-12-epideoxoscalarin, A-80014
22,25-Epoxy-5-furostene-2α,3β,26-triol, *in* E-70015
25(27)-Spirostene-2,3,6-triol, S-70064

$C_{27}H_{42}O_6$
20-Acetoxy-2α-angeloyloxy-7,14-labdadiene-3α,13*R*-diol, *in* L-80007
20-Acetoxy-2α-angeloyloxy-8(17),14-labdadiene-7α,13*R*-diol, *in* L-80008
Lucidenic acid *M*, L-60037

$C_{27}H_{42}O_7$
3α-Acetoxy-2α-angeloyloxy-8β,20-epoxy-14-labdene-7α,13*R*-diol, *in* E-80036
20-Acetoxy-2α-angeloyloxy-8(17),14-labdadiene-3α,7α,13*R*-triol, *in* L-80006

$C_{27}H_{42}O_{13}$
Jasmesoside, *in* J-80004

$C_{27}H_{42}O_{14}$
9″-Hydroxyjasmesoside, *in* J-80004

$C_{27}H_{42}O_{15}$
Penstebioside, P-60016

$C_{27}H_{44}O$
(24*S*,25*S*)-24,26-Cyclo-5α-cholest-22*E*-en-3β-ol, *in* P-60004
Trisnorisoespinenoxide, T-80368

$C_{27}H_{44}O_2$
Astrogorgiadiol, A-80181
Cholesta-7,22-diene-3,6-diol, C-80124
3-Hydroxy-25,26,27-trisnor-24-cycloartanal, H-60232
24-Methyl-27-nor-7,22-cholestadiene-3,6-diol, M-80123

$C_{27}H_{44}O_3$
11-Hydroxy-3,6-cholestanedione, H-80138
Lansilactone, L-60013

$C_{27}H_{44}O_5$
Spirostane-1,2,3-triol, S-60043

$C_{27}H_{44}O_6$
22,25-Epoxy-2,3,6,26-furostanetetrol, E-70015

$C_{27}H_{44}O_7$
▷ 2,3,14,20,22,25-Hexahydroxy-7-cholesten-6-one, H-60063
3-*epi*-20-Hydroxyecdysone, *in* H-60063
Pterosterone, P-60192

$C_{27}H_{44}O_8$
2,3,5,14,20,22,25-Heptahydroxy-7-cholesten-6-one, H-60023

$C_{27}H_{44}O_{15}$
Confertoside, C-70193

$C_{27}H_{46}O_2$
5-Cholestene-3,26-diol, C-60147
20,29,30-Trisnor-3,19-lupanediol, T-60404
Turbinaric acid, T-80371

$C_{27}H_{46}O_3$
Cholest-5-ene-3,16,22-triol, C-70172

$C_{27}H_{47}FeN_6O_9$
Ferrioxamine D_1, *in* F-60003

$C_{27}H_{47}N_9O_{10}S_2$
Trypanothione, T-70331

$C_{27}H_{48}$
1,3,5-Triheptylbenzene, T-70246

$C_{27}H_{48}O_3$
Hipposterol, H-70091

$C_{27}H_{48}O_7$
Cholestane-3,6,7,8,15,16,26-heptol, C-80125

$C_{27}H_{54}$
13-Heptacosene, H-60019

$C_{27}H_{56}$
2-Methylhexacosane, M-80095

$C_{28}H_{12}N_2O_2$
Flavanthrone, F-80010

$C_{28}H_{14}$
Benzo[*a*]coronene, B-60021
[7]Circulene, C-80134

$C_{28}H_{14}O_2$
Dibenzo[*fg,ij*]pentaphene-15,16-dione, D-80073
Dibenzo[*a,j*]perylene-8,16-dione, D-70073

$C_{28}H_{14}S$
Dibenzo[2,3:10,11]perylo[1,12-*bcd*]thiophene, D-70074

$C_{28}H_{16}O$
Diphenanthro[2,1-*b*:1′,2′-*d*]furan, D-70470
Diphenanthro[9,10-*b*:9′,10′-*d*]furan, D-70471

$C_{28}H_{17}N$
9*H*-Tetrabenzo[*a,c,g,i*]carbazole, T-70011

$C_{28}H_{18}$
Benzonaphtho[2.2]paracyclophane, B-80029
7,8-Dimethylbenzo[*no*]naphtho[2,1,8,7-*ghij*]pleiadene, D-80419

$C_{28}H_{18}O_5$
2-Benzoylbenzoic acid; Anhydride, *in* B-80054

$C_{28}H_{18}O_8$
2,2′,4,4′,7,7′,8,8′-Octahydroxy-1,1′-biphenanthrene, O-80017

$C_{28}H_{19}N$
Di-9-phenanthrylamine, D-70472

$C_{28}H_{20}$
1-Benzylidene-2,3-diphenylindene, B-80059

$C_{28}H_{20}N_2$
Tetraphenylpyrimidine, T-80159

$C_{28}H_{20}N_2O_6$
4,4′-Diamino-3,3′-biphenyldicarboxylic acid; N,N′-Dibenzoyl, *in* D-80049

$C_{28}H_{20}O_4$
2,2′-Dihydroxystilbene; Dibenzoyl, *in* D-80378
3,3,6,6-Tetraphenyl-1,4-dioxane-2,5-dione, T-60165

$C_{28}H_{22}$
5,6-Dihydro-11,12-diphenyldibenzo[*a*,*e*]cyclooctene, D-70202

$C_{28}H_{22}N_2$
9,9′-Biacridylidene; *N*,*N*′-Di-Me, *in* B-70090

$C_{28}H_{22}N_2O$
Isoamarin; 1-Benzoyl, *in* D-80263

$C_{28}H_{22}O$
2,2,4,4-Tetraphenyl-3-butenal, T-70148

$C_{28}H_{22}O_6$
Gnetin A, G-70023

$C_{28}H_{22}O_7$
Scirpusin A, S-50031

$C_{28}H_{22}O_8$
Scirpusin B, *in* S-50031
4,4′,5,5′-Tetrahydroxy-1,1′-binaphthyl; Tetra-Ac, *in* T-70102
4,4′,5,5′-Tetrahydroxy-1,1′-binaphthyl; Tetra-Ac, *in* T-80086

$C_{28}H_{22}O_{10}$
Cephalochromin, C-60029

$C_{28}H_{24}$
[2.0.2.0]Metacyclophane, M-60031

$C_{28}H_{24}N_2$
Amarin; 1-Benzyl, *in* D-80263

$C_{28}H_{24}O_4$
Isomarchantin *C*, I-60107
Isoriccardin *C*, I-60135
Riccardin *D*, R-70005

$C_{28}H_{24}O_8$
Cassigarol *A*, C-70025

$C_{28}H_{24}O_{13}$
Isoorientin; 2″-(4-Hydroxybenzoyl), *in* I-80068

$C_{28}H_{26}O_{16}$
Taxillusin, *in* P-70027

$C_{28}H_{28}O_4$
2α,6α,11-Trihydroxy-7,9(11),13-abietatrien-12-one, *in* D-70282

$C_{28}H_{28}O_{11}$
Dukunolide *C*, *in* D-60522

$C_{28}H_{28}O_{15}$
ε-Rhodomycinone; 7-Glucoside, *in* R-70002

$C_{28}H_{30}O_{10}$
Physalin *G*, P-60146

$C_{28}H_{30}O_{15}$
7-Hydroxy-3′,4′-methylenedioxyisoflavone; *O*-Laminarabioside, *in* H-80203

$C_{28}H_{30}O_{16}$
3′,4′,5,7-Tetrahydroxyisoflavone; 3′,4′-Methylene ether, 7-*O*-glucosylglucoside, *in* T-80109

$C_{28}H_{31}N_2O_3^{\oplus}$
Rhodamine B, R-80006

$C_{28}H_{32}N_8$
3,11,19,27,33,34,35,36-Octaazapentacyclo[27.3.1.1^{5,9}.1^{13,17}.1^{21,25}]hexatriaconta-1(33),5(34),6,8,13,(35),14,16,21(36),22,24,29,31-dodecaene, O-80002

$C_{28}H_{32}O_4$
Agerasanin, A-70072

$C_{28}H_{32}O_6$
Garcinone *E*, G-60003

$C_{28}H_{32}O_9$
Physalin M, *in* P-60147

$C_{28}H_{32}O_{10}$
Glaucin *B*, G-70017
Physalin L, P-60147

$C_{28}H_{32}O_{11}$
Physalin *D*, P-60145

$C_{28}H_{32}O_{13}$
7-Hydroxy-4′-methoxyisoflavone; 7-*O*-Rhammosylglucoside, *in* H-80190
7-Hydroxy-4′-methoxyisoflavone; 7-*O*-Rutinoside, *in* H-80190
Picropodophyllin glucoside, *in* P-80165
Podophyllotoxin; 1-β-D-Glucoside, *in* P-80165

$C_{28}H_{32}O_{14}$
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-Rhamnosylglucoside, *in* D-80337
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-Rutinoside, *in* D-80337
Fortunellin, *in* D-70319
7-Hydroxy-4′-methoxyisoflavone; 7-*O*-Laminarabioside, *in* H-80190
Linarin, *in* D-70319

$C_{28}H_{32}O_{15}$
Abrusin 2″-*O*-apioside, *in* A-80004
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-Gentiobioside, *in* D-80337
Flavocommelin, *in* S-80052
Kakkalide, *in* T-80112
3′,4′,7-Trihydroxyisoflavone; 4′-Me ether, 7-*O*-rhamnosylglucoside, *in* T-80308

$C_{28}H_{32}O_{16}$
3′-*O*-Methyllutonarin, *in* I-80068
4′,5,7-Trihydroxy-6-methoxyisoflavone; 7-*O*-Gentobioside, *in* T-80319

$C_{28}H_{34}O_4$
Balaenonol, *in* B-70006

$C_{28}H_{34}O_5$
Azadiradione, A-70281
Encecanescin, E-70008
9′-Epiencecanescin, *in* E-70008

$C_{28}H_{34}O_7$
▷ Gedunin, G-70006
Withaphysalin *E*, W-60009

$C_{28}H_{34}O_8$
Drummondin F, D-80533
6α-Hydroxygedunin, *in* G-70006

$C_{28}H_{34}O_9$
4-*O*-*Demethylmicrophyllinic acid*, *in* M-70147

$C_{28}H_{34}O_{10}$
Flavaspidic acids; Di-Ac, *in* F-80011
Gomisin *D*, G-70025

$C_{28}H_{34}O_{11}$
6β,9α,14-Triacetoxy-1α-benzoyloxy-4β-hydroxy-8-oxodihydro-β-agarofuran, *in* E-60018

$C_{28}H_{34}O_{13}$
1-Acetoxypinoresinol 4′-*O*-β-D-glucopyranoside, *in* H-60221

$C_{28}H_{35}ClO_{11}$
Junceellin, J-80014

$C_{28}H_{35}ClO_{12}$
Praelolide, *in* J-80014

$C_{28}H_{36}N_2O_6$
Sarcodictyin *A*, S-70010

$C_{28}H_{36}O_3$
Balaenol, B-70006

$C_{28}H_{36}O_4$
Daturilin, D-60003
Isobalaendiol, *in* B-70006
Isowithametelin, *in* W-80004
Withametelin, W-60005
Withametelin, W-80004

$C_{28}H_{36}O_5$
Celastanhydride, C-70028
2,3-Dihydroxy-6-oxo-23,24-dinor-1,3,5(10),7-friedelatetraen-29-oic acid, D-80351

$C_{28}H_{36}O_6$
Jaborol, J-60001

$C_{28}H_{36}O_7$
▷ 1,2-Dihydrogedunin, *in* G-70006
Trechonolide *A*, T-60227

$C_{28}H_{36}O_8$
3-[3-Acetyl-5-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxybenzyl]-4-hydroxy-5-methyl-6-propyl-2*H*-pyran-2-one, *in* A-80021

$C_{28}H_{36}O_{10}$
Rzedowskin *A*, R-70016
6β,9β,15-Triacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran, *in* P-80032

$C_{28}H_{36}O_{11}$
6β,9α,14-Triacetoxy-1α-benzoyloxy-4β,8β-dihydroxydihydro-β-agarofuran, *in* E-60018

$C_{28}H_{36}O_{16}$
Shanzhiside; 6-(4-Hydroxy-3,5-dimethoxybenzoyl), 8-Ac, Me ester, *in* S-60028

$C_{28}H_{37}ClO_{10}$
Ptilosarcone, *in* P-60195

$C_{28}H_{38}N_2O_{10}$
1,2-Bis(4′-benzo-15-crown-5)diazene, B-60141

$C_{28}H_{38}N_4O_6$
Chlamydocin, C-60038

$C_{28}H_{38}O_4$
Cystoketal, C-60234
Isocystoketal, *in* C-60234

$C_{28}H_{38}O_5$
Daturilinol, D-70007
Mzikonone, M-70166
Withacoagin, W-80003

$C_{28}H_{38}O_7$
Physanolide, P-60149
Withanolide *Y*, W-60007
Withaphysanolide, W-60010

$C_{28}H_{38}O_9$
3,14-Diacetoxy-2-butanoyloxy-5,8(17)-briaradien-18,7-olide, *in* E-70012
4,14-Diacetoxy-2-butanoyloxy-5,8(17)-briaradien-18,7-olide, *in* E-70012
ent-2α,3α,6β,11β-Tetraacetoxy-16-kauren-15-one, *in* P-80047
Xenicin, X-70004

$C_{28}H_{38}O_{10}$
Ingol; Tetra-Ac, *in* I-70018
Lapidolinin, *in* L-60015
ent-2α,3α,6β,11β-Tetraacetoxy-7β-hydroxy-16-kauren-15-one, *in* P-80047

$C_{28}H_{38}O_{11}$
Junceellolide D, J-80017

$C_{28}H_{39}ClO_8$
Physalolactone, P-60148

$C_{28}H_{39}ClO_{10}$
Ptilosarcol, P-60195

$C_{28}H_{39}NO$
Emindole SA, *in* E-60005
Emindole DA, E-60005

$C_{28}H_{40}$
24,25-Dinor-1,3,5(10),12-oleanatetraene, D-80497
24,25-Dinor-1,3,5(10),12-ursatetraene, D-80498
1,3,5,7-Tetra-*tert*-butyl-*s*-indacene, T-60025
Tetrakis(cyclohexylidene)cyclobutane, T-80130

$C_{28}H_{40}O_2$
Plastoquinone 4, P-80159

$C_{28}H_{40}O_3$
11′-Methoxysargaquinone, *in* S-60010
9′-Methoxysargaquinone, *in* S-60010

$C_{28}H_{40}O_4$
8′,9′-Dihydroxy-5-methylsargaquinone, *in* S-60010

$C_{28}H_{40}O_5$
Amentol 1′-methyl ether, *in* A-60088
Balearone, B-60005
Bifurcarenone; 2′-Me ether, *in* B-80093
Epineobalearone, *in* N-80018
12-Hydroxy-24-methyl-24-oxo-16-scalarene-22,25-dial; O^{12}-Ac, *in* H-60191
Isobalearone, *in* B-60005
Neobalearone, N-80018
Strictaepoxide, S-60056
Strictaketal, S-70076

$C_{28}H_{40}O_6$
Ixocarpanolide, I-60143

$C_{28}H_{40}O_7$
6α,7α-Epoxy-5α,14α,20*R*-trihydroxy-1-oxo-22*R*,24*S*,25*R*-with-2-enolide, *in* I-60143
Jaborosalactol N, J-80002
Jaborosalactone *M*, *in* J-80001
Withaphysacarpin, W-60008

$C_{28}H_{40}O_9$
Astrogorgin, A-80182

$C_{28}H_{40}O_{13}$
Bonafousioside, B-80171

$C_{28}H_{41}ClO_9$
Solenolide A, S-70052

$C_{28}H_{42}$
24,25-Dinor-1,3,5(10)-lupatriene, D-80496

$C_{28}H_{42}O_4$
Maesol, M-80002

$C_{28}H_{42}O_5$
16β-Acetoxy-24-methyl-12,24-dioxo-25-scalaranal, *in* H-80200
Tubocapsigenin *A*, T-70333

$C_{28}H_{42}O_6$
11,15(17)-Trinervitadiene-3,9,13-triol; 9-Ac, 3,13-dipropanoyl, *in* T-70297

$C_{28}H_{42}O_7$
Jaborosalactol *M*, J-80001

$C_{28}H_{44}O$
24-Methyl-7,22-cholestadien-3-one, *in* M-80059
24-Methyl-5,22,25-cholestatrien-3-ol, M-60057

$C_{28}H_{44}O_{11}$
Grayanoside *A*, *in* G-80038

$C_{28}H_{46}O$
24-Methyl-7,22-cholestadien-3-ol, M-80059

$C_{28}H_{46}O_2$
24-Methyl-7,22-cholestadiene-3,6-diol, M-80058
4-Methylcholesta-8,14-dien-23-ol, M-80060
Phytylplastoquinone, P-80144

$C_{28}H_{46}O_3$
24-Methyl-7,22-cholestadiene-3,5,6-triol, M-70057

$C_{28}H_{46}O_4$
24-Methylene-5-cholestene-3,4,7,20-tetrol, M-60070

$C_{28}H_{46}O_5$
Dolichosterone, D-70544
22*S*,25-Epoxy-24-methyl-3,11,20-furostanetriol, E-80039

$C_{28}H_{46}O_6$
2-Desacetyl-22-epihippurin 1, *in* E-80039
2α-Hydroxyhippuristanol, *in* E-80039

$C_{28}H_{46}O_7$
Polypodoaurein, *in* H-60063

$C_{28}H_{47}N_9O_9$
Neokyotorphin, N-70025

$C_{28}H_{48}O_3$
24-Methyl-7-cholestene-3,5,6-triol, M-80061
β-Tocopherol, T-80200
γ-Tocopheryl quinone, T-80201

$C_{28}H_{48}O_4$
6-Deoxodolichosterone, *in* D-70544
Numersterol A, N-80084
3α,22*R*,23*R*-Trihydroxy-24*S*-methyl-5α-cholestan-6-one, *in* T-70116

$C_{28}H_{48}O_5$
2,3,22,23-Tetrahydroxy-24-methyl-6-cholestanone, T-70116

$C_{28}H_{48}O_6$
Brassinolide, B-70178

$C_{28}H_{48}O_{12}$
4,7,10,15,18,21,24,27,30,33,36,39-Dodecaoxatricyclo[11.9.9.$9^{2,12}$]tetraconta-1,12-diene, D-70535

$C_{28}H_{50}O_4$
6-Deoxocastasterone, *in* T-70116

$C_{28}H_{52}O_3$
Ficulinic acid B, F-60012

$C_{28}H_{52}O_{11}$
Muricatin B, *in* H-80172

$C_{28}H_{56}O$
Octacosanal, O-80005

$C_{28}H_{58}$
3-Methylheptacosane, M-80092

$C_{29}H_{18}O$
Di-9-anthracenylmethanone, D-60050

$C_{29}H_{20}$
7,7-Diphenylbenzo[*c*]fluorene, D-70473
Tetrabenzotetracyclo[5.5.1.$0^{4,13}$.$0^{10,13}$]tridecane, T-60019

$C_{29}H_{22}$
1,2,3,4-Tetraphenylcyclopentadiene, T-70149

$C_{29}H_{22}O$
1,1,5,5-Tetraphenyl-1,4-pentadien-3-one, T-80158

$C_{29}H_{22}O_{14}$
3,5-Digalloylepicatechin, *in* P-70026

$C_{29}H_{24}O_{10}$
Chaetochromin *C*, *in* C-60029

$C_{29}H_{24}O_{15}$
4′,5,6,7-Tetrahydroxyisoflavone; 6,7-Di-Me ether, 4′-*O*-rhamnosylglucoside, *in* T-80112

$C_{29}H_{26}O_4$
Riccardin *E*, *in* R-70005

$C_{29}H_{28}O_4$
Tetrabenzyloxymethane, *in* M-80037

$C_{29}H_{28}O_{10}$
Di-2-(7-acetyl-1,4-dihydro-3,6,8-trihydroxy-4,4-dimethyl-1-oxonaphthyl)methane, D-80043

$C_{29}H_{28}O_{12}$
Viscutin 2, *in* T-60103

$C_{29}H_{29}N_3O_8$
K 13, K-70001

$C_{29}H_{30}O_7$
8-Prenyllepidissipyrone, *in* L-80023

$C_{29}H_{32}O_{12}$
Amorphigenin; *O*-β-D-Glucopyranoside, *in* A-80152

$C_{29}H_{32}O_{16}$
Irisolone-4′-bioside, *in* D-80341
3′,4′,6,7-Tetrahydroxyisoflavone; 6-Me, 3′,4′-methylenedioxy ether, 7-*O*-laminarabioside, *in* T-80111

$C_{29}H_{34}O_7$
Triptofordin *B*, T-60393

$C_{29}H_{34}O_8$
Nimbanal, N-80026

$C_{29}H_{34}O_{10}$
Crepiside *A*, *in* Z-60001
Crepiside *B*, *in* Z-60001

$C_{29}H_{34}O_{11}$
Ixerin C, *in* I-80102
Physalin *I*, *in* P-60145
Trijugin *A*, T-60351

$C_{29}H_{34}O_{12}$
Acetoxyeumaitenol, *in* E-60072
Dalpanol; *O*-Glucoside, *in* D-80003

$C_{29}H_{34}O_{13}$
Amorphigenol glucoside, *in* A-80152

$C_{29}H_{34}O_{14}$
Embinin, *in* S-80052
Pueroside *A*, *in* P-70137

$C_{29}H_{34}O_{15}$
4′,7,8-Trihydroxyisoflavone; 4′,8-Di-Me ether, 7-*O*-laminarabioside, *in* T-80311

$C_{29}H_{34}O_{16}$
4′,5,6,7-Tetrahydroxyisoflavone; 6,7-Di-Me ether, 4′-*O*-[4-*O*-β-D-glucopyranosyl (1→4)-β-D-glucopyranoside], *in* T-80112

$C_{29}H_{36}O_6$
Demethylzeylasteral, *in* D-70027

$C_{29}H_{36}O_7$
Desmethylzeylasterone, D-70027

$C_{29}H_{36}O_8$
Fissinolide, *in* S-80054

$C_{29}H_{36}O_9$
3-Acetylswietenolide, *in* S-80054
Microphyllinic acid, M-70147

$C_{29}H_{36}O_{10}$
Baccharinoid B27, *in* B-60002

$C_{29}H_{36}O_{13}$
1-Hydroxypinoresinol; 4″-Me ether, 1-Ac, 4′-*O*-β-D-glucopyranoside, *in* H-60221

$C_{29}H_{36}O_{16}$
Olivin 4-diglucoside, *in* O-80043

$C_{29}H_{37}NO_3$
Smenospongidine, *in* S-80036

$C_{29}H_{38}N_2O_6$
Sarcodictyin *B*, *in* S-70010

$C_{29}H_{38}O_5$
23-Nor-6-oxopristimerol, *in* D-80351

$C_{29}H_{38}O_7$
Isonimolide, I-60110
Trechonolide *B*, *in* T-60227

$C_{29}H_{38}O_9$
▷ Roridin *D*, R-70008
Scutellone *A*, S-60017
Scutellone *C*, S-70019
Scuterivulactone C_2, *in* S-60017

$C_{29}H_{38}O_{10}$
Baccharinoid B9, B-60001
Baccharinoid B13, B-60002
Baccharinoid B16, B-60003
Baccharinoid B10, *in* B-60001
Baccharinoid B12, *in* R-70008
Baccharinoid B14, *in* B-60002
Baccharinoid B17, *in* R-70008
Baccharinoid B21, *in* R-70008

$C_{29}H_{38}O_{11}$
Baccharinol, B-70003
Isobaccharinol, *in* B-70003

$C_{29}H_{40}O_5$
Secowithametelin, S-80019

$C_{29}H_{40}O_8$
Physalactone, P-60144

$C_{29}H_{40}O_9$
Ingol; 3,7-Di-Ac, 12-tigloyl, *in* I-70018

$C_{29}H_{40}O_{10}$
Baccharinoid *B*1, B-70001
Baccharinoid *B*7, B-70002
Baccharinoid **B2**, *in* B-70001

Baccharinoid **B3**, *in* B-70002
Baccharinoid B20, *in* B-60001
Baccharinoid B23, *in* B-60003
Baccharinoid B24, *in* B-60003

$C_{29}H_{42}O_3$
Bryophollone, B-80271

$C_{29}H_{42}O_4$
Przewanoic acid *B*, P-70126
15Z-Cinnamoyloxy-7-labden-17-oic acid, *in* H-80183

$C_{29}H_{42}O_5$
Zosterondiol B, Z-80005

$C_{29}H_{42}O_7$
3α,20-Diacetoxy-2α-angeloyloxy-9α,13*R*-epoxy-7,14-labdadiene, *in* E-80035

$C_{29}H_{42}O_{11}$
Ghalakinoside, G-80016

$C_{29}H_{44}O_2$
3β-Hydroxy-28-noroleana-12,17-dien-16-one, *in* M-70011

$C_{29}H_{44}O_3$
3-Hydroxy-30-nor-12,18-oleanadien-29-oic acid, H-80218
3-Hydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, H-60199
18β-Hydroxy-28-nor-3,16-oleanenedione, *in* D-60363

$C_{29}H_{44}O_4$
3,23-Dihydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, D-70324
3,24-Dihydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, D-80344
Kanerin, K-80001

$C_{29}H_{44}O_5$
Floridic acid, F-80014
Zosterdiol A, Z-80003
Zosterdiol B, Z-80004
Zosterondiol A, *in* Z-80005
Zosteronol, *in* Z-80004

$C_{29}H_{44}O_6$
Brachycarpone, B-60195
Heteronemin, H-60030
11,15(17)-Trinervitadiene-3,9,13-triol; 3,9,13-Tripropanoyl, *in* T-70297

$C_{29}H_{44}O_8$
3α,20-Diacetoxy-2α-angeloyloxy-8,14-labdadiene-7α,13*R*-diol, *in* L-80005
3α,20-Diacetoxy-2α-angeloyloxy-8(17),14-labdadiene-7α,13*R*-diol, *in* L-80006

$C_{29}H_{44}O_9$
Coroglaucigenin; 3-*O*-Rhamnoside, *in* C-60168
▷ Frugoside, *in* C-60168
Methyl 15α,17β-diacetoxy-6α-butanoyloxy-15,16-dideoxy-15,17-oxido-16-spongianate, *in* T-60038

$C_{29}H_{45}N_3O_3$
Blastmycetin *D*, B-60191

$C_{29}H_{46}O_2$
Maragenin I, M-70011

$C_{29}H_{46}O_3$
3,18-Dihydroxy-28-nor-12-oleanen-16-one, D-60363

$C_{29}H_{46}O_4$
Baccatin, B-80001

$C_{29}H_{46}O_7$
2α,7α-Diacetoxy-6β-isovaleroyloxy-8,13*E*-labdadien-15-ol, *in* L-60002

$C_{29}H_{46}O_8$
Viticosterone *E*, *in* H-60063

$C_{29}H_{47}N_5O_5$
Stacopin P1, S-60051

$C_{29}H_{47}N_5O_6$
Stacopin P2, *in* S-60051

$C_{29}H_{48}O$
Ficisterol, F-60010
Hebesterol, H-60011

$C_{29}H_{48}O_2$
24,25-Epoxy-29-nor-3-cycloartanol, E-70026
29-Nor-23-cycloartene-3,25-diol, N-70073
28-Nor-16-oxo-17-oleanen-3β-ol, *in* M-70011

$C_{29}H_{48}O_3$
24-Ethyl-7,22-cholestadiene-3,5,6-triol, E-80060
24-Ethylidene-7-cholestene-3,5,6-triol, E-80066
6β-Methoxy-7,22-ergostadiene-3β,5α-diol, *in* M-70057
29-Nor-8,24-lanostadiene-1,2,3-triol, N-80081

$C_{29}H_{50}O$
Petrostanol, P-60066

$C_{29}H_{50}O_2$
24-Ethyl-7-cholestene-3,6-diol, E-80061
4-Stigmastene-3,6-diol, S-60054

$C_{29}H_{50}O_3$
24,24-Dimethoxy-25,26,27-trisnor-3-cycloartanol, *in* H-60232
Numersterol B, N-80085

$C_{29}H_{50}O_4$
24(28)-Stigmastene-2,3,22,23-tetrol, S-70075

$C_{29}H_{52}N_{10}O_6$
Argiopine, A-60295

$C_{29}H_{52}O$
24,24-Dimethyl-3-cholestanol, D-70389

$C_{29}H_{52}O_2$
3,6-Stigmastanediol, S-70074

$C_{29}H_{58}O$
15-Nonacosanone, N-80066

$C_{29}H_{60}$
2-Methyloctacosane, M-80124

$C_{29}H_{60}O$
15-Nonacosanol, N-80064
1-Nonacosanol, N-80065

$C_{30}H_{14}$
[5]Phenylene, P-60090

$C_{30}H_{16}$
Pyranthrene, P-70151
Tribenzo[*b,n,pqr*]perylene, T-60244

$C_{30}H_{16}O_2$
7,16-Heptacenedione, H-60018

$C_{30}H_{18}$
Di-9-anthrylacetylene, D-60051

$C_{30}H_{18}O_8$
Siameanin, S-80031

$C_{30}H_{18}O_9$
Cassianin, *in* S-80031
Roseoskyrin, R-80011

$C_{30}H_{18}O_{10}$
Hinokiflavone, H-60082
Rhodoislandin A, R-80007
Rhodoislandin B, R-80008

$C_{30}H_{18}O_{12}$
Bryoflavone, B-70283
Dicranolomin, D-70144
Heterobryoflavone, H-70027

$C_{30}H_{20}$
1,2,3-Triphenylcyclopent[*a*]indene, T-70306

$C_{30}H_{20}O_4$
Tetrabenzoylethylene, T-60021

$C_{30}H_{20}O_9$
1-[3-(2,4-Dihydroxybenzoyl)-4,6-dihydroxy-2-(4-hydroxyphenyl)-7-benzofuranyl]-3-(4-hydroxyphenyl)-2-propen-1-one, D-70286

$C_{30}H_{20}O_{11}$
2,3-Dihydro-3′,4′,4″,5,5″,7,7″-heptahydroxy-3,8′-biflavone, D-80209

$C_{30}H_{20}O_{12}$
2,3-Dihydrodicranolomin, *in* D-70144

$C_{30}H_{20}S_2$
1,3,4,6-Tetraphenylthieno[3,4-*c*]thiophene-5-S^{IV}, T-70152

$C_{30}H_{20}S_8$
Tetramercaptotetrathiafulvalene; Tetrakis (*S*-Ph), *in* T-70130

$C_{30}H_{22}N_4O_4$
6,6′-(1,2-Dimethyl-1,2-ethanediyl)bis[1-phenazinecarboxylic acid], D-70411

$C_{30}H_{22}O_4$
1,1,2,2-Tetrabenzoylethane, T-60020

$C_{30}H_{22}O_7$
Palmidin B, P-80005
Palmidin C, *in* P-80005

$C_{30}H_{22}O_8$
Aloeemodin dianthrone, A-80049
Lophirone *A*, L-60035
Lophirone B, L-80037
Lophirone C, L-80038
Palmidin A, *in* P-80005

$C_{30}H_{22}O_9$
Daphnodorin *D*, D-70005
1-[3-(2,4-Dihydroxybenzoyl)-4,6-dihydroxy-2-(4-hydroxyphenyl)-7-benzofuranyl]-3-(4-hydroxyphenyl)-2-propen-1-one; 2,3-Dihydro (trans-), *in* D-70286
Maackiasin, M-60001

$C_{30}H_{22}O_{10}$
GB1a, *in* G-70005
Isochamaejasmin, I-70064

$C_{30}H_{22}O_{11}$
GB 1, G-70005
GB2a, *in* G-70005

$C_{30}H_{22}O_{12}$
3″,3‴,4′,4‴,5,5″,7,7″-Octahydroxy-3,8″-biflavanone, *in* G-70005

$C_{30}H_{22}O_{13}$
Chiratanin, C-60037

$C_{30}H_{24}N_6O_3$
Furlone yellow, F-70053

$C_{30}H_{24}O_4$
Tecomaquinone I, T-60010

$C_{30}H_{24}O_9$
Shiraiachrome C, S-80030

$C_{30}H_{24}O_{10}$
Chaetochromin *D*, *in* C-60029
Mahuannin A, M-80003
Mahuannin B, *in* M-80003

$C_{30}H_{24}O_{13}$
[2′,2′]-Catechin-taxifolin, C-60023

$C_{30}H_{26}O_5$
Tecomaquinone III, T-70006

$C_{30}H_{26}O_6$
Flavanthrin, F-70011

$C_{30}H_{26}O_8$
Isombamichalcone, *in* M-70014
Mbamichalcone, M-70014

$C_{30}H_{26}O_{10}$
Chaetochromin, *in* C-60029
Chaetochromin *B*, *in* C-60029
Shiraiachrome A, S-80028
Shiraiachrome B, S-80029

$C_{30}H_{28}N_4O_2$
Tetrahydro-1,2,4,5-tetrazine-3,6-dione; 1,2,4,5-Tetrabenzyl, *in* T-70097

$C_{30}H_{28}O_6$
Angoluvarin, A-70208
Isothamnosin A, I-70104
Isothamnosin B, *in* I-70104

$C_{30}H_{28}S_2$
2,18-Dithia[3.1.3.1]paracyclophane, D-80518

$C_{30}H_{30}O_7$
Euchretin A, E-80080

$C_{30}H_{30}O_8$
▷ Gossypol, G-60032

$C_{30}H_{30}O_{10}$
Phleichrome, P-70098

$C_{30}H_{30}O_{14}$
Safflomin C, S-80001

$C_{30}H_{32}O_4$
4,15,26-Tricontatrien-1,12,18,29-tetrayne-3,14,17,28-tetrone, *in* P-70044

$C_{30}H_{32}O_6$
Fruticolide, F-70045

$C_{30}H_{32}O_{14}$
Senburiside II, S-70033

$C_{30}H_{34}O_5$
Euchrenone b_1, E-70058

$C_{30}H_{34}O_6$
Eucrenone b_2, *in* E-70058

$C_{30}H_{34}O_{10}$
Cerberalignan D, C-80033
Cerberalignan E, C-80034

$C_{30}H_{34}O_{11}$
Ainsliaside *A*, *in* Z-60001

$C_{30}H_{34}O_{17}$
Platycarpanetin 7-*O*-laminaribioside, *in* P-80045

$C_{30}H_{36}O_5$
Amorilin, A-80151

$C_{30}H_{36}O_8$
Artelein, A-60303

$C_{30}H_{36}O_9$
6α-Acetoxygedunin, *in* G-70006
11β-Acetoxygedunin, *in* G-70006
Isonimolicinolide, I-60109

$C_{30}H_{36}O_{11}$
Cerberalignan F, C-80035
Cerberalignan G, *in* C-80035
Isonimbinolide, I-70072

$C_{30}H_{36}O_{12}$
Tectoroside, T-80003

$C_{30}H_{36}O_{15}$
Pueroside *B*, *in* P-70137

$C_{30}H_{36}O_{16}$
3′,4′,6,7-Tetrahydroxyisoflavone; 3′,4′,6-Tri-Me ether, *O*-laminaribioside, *in* T-80111

$C_{30}H_{37}N_5O_5$
Avellanin *B*, A-60324

$C_{30}H_{38}O_4$
Cochloxanthin, C-60156
Helilupulone, H-80008

$C_{30}H_{38}O_5$
23-Oxoisopristimerin III, *in* I-70083

$C_{30}H_{38}O_6$
Biperezone, B-80105
Caleamyrcenolide, C-80010
Zeylasteral, *in* D-70027

$C_{30}H_{38}O_7$
Furanoganoderic acid, F-80088
3,7,11,15,23-Pentaoxo-8,20*E*-lanostadien-26-oic acid, *in* D-80390

$C_{30}H_{38}O_9$
2′-O-Methylmicrophyllinic acid, in M-70147
Isolimbolide, I-60105

$C_{30}H_{38}O_{10}$
Swietemahonin A, S-80053

$C_{30}H_{38}O_{12}$
6β,8β,9α,14-Tetraacetoxy-1α-benzoyloxy-4β-hydroxydihydro-β-agarofuran, *in* E-60018

$C_{30}H_{38}O_{13}$
Bruceanol *C*, B-70280

$C_{30}H_{40}O_4$
4,5-Dihydro-6-hydroxy-3-oxo-8′-apo-ε-caroten-8′-oic acid, *in* C-60156
Isopristimerin III, I-70083
Petrosynol, P-70044

$C_{30}H_{40}O_5$
Helisplendidilactone, H-80010

$C_{30}H_{40}O_7$
15α-Hydroxy-3,7,11,23-tetraoxo-8,20*E*-lanostadien-26-oic acid, *in* D-80390
3β-Hydroxy-7,11,15,23-tetraoxo-8,20*E*-lanostadien-26-oic acid, *in* D-80390
7β-Hydroxy-3,11,15,23-tetraoxo-8,20(22)-lanostadien-26-oic acid, *in* T-70254

$C_{30}H_{40}O_8$
7,12-Dihydroxy-3,11,15,23-tetraoxo-8,20(22)-lanostadien-26-oic acid, D-60378
Ganoderic acid *O*, *in* D-60379
Trichilinin, T-60251
Withaminimin, W-60006

$C_{30}H_{40}O_{10}$
1,2-Bis(4′-benzo-15-crown-5)ethene, B-60142
Xenicin; 9-Deacetyl, 9-acetoacetyl, *in* X-70004

$C_{30}H_{41}ClO_{10}$
Brianthein V, B-80172

$C_{30}H_{42}O_3$
Heleniumlactone 1, H-60013
Heleniumlactone 3, H-60014
Heleniumlactone 2, *in* H-60013

$C_{30}H_{42}O_4$
Firmanolide, F-60013
Isomaresiic acid *C*, I-60108
Mariesiic acid *C*, M-60011

$C_{30}H_{42}O_5$
Abiesonic acid, A-60005

$C_{30}H_{42}O_7$
Bufalin; 3-(Hydrogen adipoyl), *in* B-70289
▷ Cucurbitacin *I*, *in* C-70204
3,15-Dihydroxy-7,11,23-trioxo-8,20-lanostadien-26-oic acid, D-80390
7β,15α-Dihydroxy-3,11,23-trioxo-8,20(22)*E*-lanostadien-26-oic acid, *in* T-70254
3β,7β-Dihydroxy-11,15,23-trioxo-8,20(22)*E*-lanostadien-26-oic acid, *in* T-70254

$C_{30}H_{42}O_8$
7,20-Dihydroxy-3,11,15,23-tetraoxo-8-lanosten-26-oic acid, D-60379
Proscillaridin *A*, *in* B-70289

$C_{30}H_{42}O_9$
Ingol; 7-Angeloyl, O^8-Me, 3,12-Di-Ac, *in* I-70018
Ingol; 7-Tigloyl, O^8-Me, 3,12-di-Ac, *in* I-70018
12,15,20-Trihydroxy-3,7,11,23-tetraoxo-8-lanosten-26-oic acid, T-80340

$C_{30}H_{42}O_{10}$
Kopeoside, *in* K-80012

$C_{30}H_{42}O_{12}$
Baccatin I; 5-Deacetyl, *in* B-80002
1-Dehydroxy-4-deacetylbaccatin IV, *in* B-80003

$C_{30}H_{43}NO_6$
Bisparthenolidine, B-80157

$C_{30}H_{44}O_4$
3,23-Dioxo-7,24-lanostadien-26-oic acid, D-60472
3,23-Dioxo-7,25(27)-lanostadien-26-oic acid, *in* D-60472
3,7-Dioxo-12-oleanen-28-oic acid, D-70469
23-Oxomariesiic acid *A*, *in* M-70012
23-Oxomariesiic acid *B*, *in* M-60010

$C_{30}H_{44}O_5$
Abrusogenin, A-80005
Chiisanogenin, C-70038
3,15-Dihydroxy-23-oxo-7,9(11),24-lanostatrien-26-oic acid, D-70330
2,19-Dihydroxy-3-oxo-1,12-ursadien-28-oic acid, D-80352

$C_{30}H_{44}O_6$
11-Deoxocucurbitacin *I*, *in* C-70204
9,11-Dihydro-22,25-oxido-11-oxoholothurinogenin, D-70237

$C_{30}H_{44}O_7$
▷ Cucurbitacin *D*, C-70203
Cucurbitacin *L*, *in* C-70204
3,7,15-Trihydroxy-11,23-dioxo-8,20(22)-lanostadien-26-oic acid, T-70254

$C_{30}H_{44}O_{10}$
Perusitin, *in* C-80017

$C_{30}H_{46}O$
9(11),12-Oleanadien-3-one, O-60032

$C_{30}H_{46}O_2$
21,23-Epoxy-7,24-tirucalladien-3-one, *in* E-60032
21-Hopene-3,20-dione, H-80097

$C_{30}H_{46}O_3$
24*S*,25*S*-Epoxy-26-hydroxy-7,9(11)-lanostadien-3-one, *in* E-70025
Flindissol lactone, *in* F-70013
Flindissone, *in* F-70013
28-Hydroxy-20(29)-lupene-3,7-dione, H-80185
3-Hydroxy-12-oleanen-29,22-olide, H-70197
7-Hydroxy-3-oxo-8,24-lanostadien-26-al, H-70200
22-Hydroxy-7,24-tirucalladiene-3,23-dione, H-70227
3-Oxo-24-cycloarten-21-oic acid, O-80072
3-Oxo-8,24-lanostadien-21-oic acid, O-80087
3-Oxo-8,24-lanostadien-26-oic acid, O-70096
3-Oxo-8-lanosten-26,22-olide, *in* H-60169
Swertialactone *C*, *in* S-60064
Swertialactone *D*, S-60064

$C_{30}H_{46}O_4$
Abiesolidic acid, A-70003
Colubrinic acid, C-70190
3,15-Dihydroxy-7,9(11),24-lanostatrien-26-oic acid, D-70314
2,3-Dihydroxy-12,20(30)-ursadien-28-oic acid, D-60381
Dumortierigenin, D-80536
12-Hydroxy-3-oxo-28,13-oleananolide, H-70201
3-Hydroxy-23-oxo-12-oleanen-28-oic acid, H-80230
19α-Hydroxy-3-oxo-12-oleanen-28-oic acid, *in* D-70327
22-Hydroxy-3-oxo-12-ursen-30-oic acid, H-70202
19α-Hydroxy-3-oxo-12-ursen-28-oic acid, *in* D-70350
Manwuweizic acid, M-70010
Mariesiic acid *A*, M-70012
Mariesiic acid *B*, M-60010
Przewanoic acid *A*, P-70125
3,4-Seco-4(28),20,24-dammaratrien-3,26-dioic acid, S-70021
15,26,27-Trihydroxy-7,9(11),24-lanostatrien-3-one, T-60330

$C_{30}H_{46}O_5$
Cadambagenic acid, C-70002
19,29-Dihydroxy-3-oxo-12-oleanen-28-oic acid, D-70331
22,23-Dihydroxy-3-oxo-12-ursen-30-oic acid, D-70333
2,3,24-Trihydroxy-13,27-cyclo-11-oleanen-28-oic acid, T-70251
2,3,24-Trihydroxy-12,27-cyclo-14-taraxeren-28-oic acid, T-70252
3,15,22-Trihydroxy-7,9(11),24-lanostatrien-26-oic acid, T-80318
2,3,24-Trihydroxy-11,13(18)-oleonadien-28-oic acid, T-60336
2α,3α,24-Trihydroxy-12,20(30)-ursadien-28-oic acid, *in* D-60381

$C_{30}H_{46}O_6$
2,3-Dihydroxy-12-oleanene-23,28-dioic acid, D-80346
3,19-Dihydroxy-12-ursene-23,28-dioic acid, D-80393

3,19-Dihydroxy-12-ursene-24,28-dioic acid, D-60382
3β,6β,19α-Trihydroxy-23-oxo-12-ursen-28-oic acid, *in* T-80129

$C_{30}H_{46}O_7$
Cucurbitacin *R*, *in* C-70203
▷ Saponaceolide A, S-60008
Saponaceolide A, S-80009
3β,6β,19α-Trihydroxy-12-ursene-23,28-dioic acid, *in* T-80129

$C_{30}H_{46}O_8$
Maquiroside *A*, *in* C-60168
Musangic acid, M-80199

$C_{30}H_{48}O$
7,9(11)-Fernadien-3-ol, F-80002
5(10)-Gluten-3-one, G-60028
14(26),17*E*,21-Malabaricatrien-3-one, *in* M-60008
30-Norcyclopterospermone, *in* N-60059
11,13(18)-Oleanadien-3-ol, O-70032
9(11),12-Oleanadien-3-ol, O-70031
9(11),12-Ursadien-3-ol, U-70007

$C_{30}H_{48}O_2$
Duryne, D-70550
11,12-Epoxy-14-taraxeren-3-ol, E-80044
21,23-Epoxy-7,24-tirucalladien-3-ol, E-60032
3-Hydroxy-20(29)-lupen-11-one, H-80186
7-Hydroxy-20(29)-lupen-3-one, H-80187
16-Hydroxy-18-oleanen-3-one, H-80223
3-Hydroxy-12-oleanen-1-one, H-80224
16β-Hydroxy-18-oleanen-3-one, *in* O-80033
11,13(18)-Oleanadiene-3,24-diol, O-80030
3-Oxo-29-friedelanal, *in* F-80082
3,4-Seco-4(23),14-taraxeradien-3-oic acid, S-60018

$C_{30}H_{48}O_3$
3β,26-Dihydroxy-5,24*E*-cucurbitadien-11-one, *in* C-60175
3β,27-Dihydroxy-5,24*Z*-cucurbitadien-11-one, *in* C-60175
24,25-Dihydroxy-7,9(11)-lanostadien-3-one, D-60343
3,23-Dihydroxy-20(30)-lupen-29-al, D-70316
1,11-Dihydroxy-20(29)-lupen-3-one, D-60345
23,30-Dihydroxy-20(29)-lupen-3-one, D-70318
1,11-Dihydroxy-18-oleanen-3-one, D-60364
24,25-Epoxy-7,9(11)-lanostadiene-3,26-diol, E-70025
Flindissol, F-70013
27-Hydroxy-3,21-friedelanedione, *in* D-70301
3-Hydroxy-8,24-lanostadien-21-oic acid, H-70152
3-Hydroxy-8-lanosten-26,22-olide, H-60169
3-Hydroxy-28,13-oleananolide, H-60200
3-Hydroxy-12-oleanen-30-oic acid, H-80222
3-Hydroxytaraxastan-28,20-olide, H-70221
3-Hydroxy-14-taraxeren-28-oic acid, H-80256
3-Hydroxy-28,20-ursanolide, H-60233
12,20(29)-Lupadiene-3,27,28-triol, L-70042
Niloticin, N-70036
3-Oxo-27-friedelanoic acid, *in* T-70218

$C_{30}H_{48}O_4$
Alisol *B*, A-70082
Careyagenolide, C-80026
3,22-Dihydroxy-24-cycloarten-26-oic acid, D-80304
3,23-Dihydroxy-24-cycloarten-26-oic acid, D-80305
3,27-Dihydroxy-24-cycloarten-26-oic acid, D-80306
3,15-Dihydroxy-8,24-lanostadien-26-oic acid, D-80331
3,23-Dihydroxy-20(29)-lupen-28-oic acid, D-70317
1,3-Dihydroxy-12-oleanen-29-oic acid, D-70325
3,19-Dihydroxy-12-oleanen-28-oic acid, D-70327
3,29-Dihydroxy-12-oleanen-28-oic acid, D-80347
3,6-Dihydroxy-12-oleanen-29-oic acid, D-70326
1,3-Dihydroxy-12-ursen-28-oic acid, D-60383
2,3-Dihydroxy-12-ursen-28-oic acid, D-70349
3,19-Dihydroxy-12-ursen-28-oic acid, D-70350
24,25-Epoxy-7,26-dihydroxy-8-lanosten-3-one, E-70013
Saikogenin *F*, S-60001
24,25,26-Trihydroxy-7,9(11)-lanostadien-3-one, *in* L-60012

$C_{30}H_{48}O_5$
Cycloorbigenin, C-60218
Squarrofuric acid, S-70070
Toosendantriol, T-60223
3,7,15-Trihydroxy-8,24-lanostadien-26-oic acid, T-60327
3,7,22-Trihydroxy-8,24-lanostadien-26-oic acid, T-60328
3,12,17-Trihydroxy-9(11)-lanosten-18,20-olide, T-70267
1,3,23-Trihydroxy-12-oleanen-29-oic acid, T-80328
2,3,23-Trihydroxy-12-oleanen-28-oic acid, T-70271
2,3,24-Trihydroxy-12-oleanen-28-oic acid, T-60335
2,3,24-Trihydroxy-12-oleanen-28-oic acid, T-80329
3β,23,27-Trihydroxy-28,20-taraxastanolide, *in* H-70221
2,3,19-Trihydroxy-12-ursen-28-oic acid, T-80342
2,3,23-Trihydroxy-12-ursen-28-oic acid, T-80343
3,11,12-Trihydroxy-20-ursen-28-oic acid, T-80344
3,19,24-Trihydroxy-12-ursen-28-oic acid, T-60348
3,19,24-Trihydroxy-12-ursen-28-oic acid, T-80345
3,6,19-Trihydroxy-12-ursen-28-oic acid, T-80346

$C_{30}H_{48}O_6$
2α-Angeloyloxy-20-(2-methylbutanoyloxy)-7,14-labdadiene-3α,13*S*-diol, *in* L-80007
3,7,15,22-Tetrahydroxy-8,24-lanostadien-26-oic acid, T-60111
2,3,19,23-Tetrahydroxy-12-oleanen-28-oic acid, T-70119
1,2,3,19-Tetrahydroxy-12-ursen-28-oic acid, T-70121
1,2,3,19-Tetrahydroxy-12-ursen-28-oic acid, T-80123
1,3,19,23-Tetrahydroxy-12-ursen-28-oic acid, T-80124
2,3,19,23-Tetrahydroxy-12-ursen-28-oic acid, T-80125
2,3,19,24-Tetrahydroxy-12-ursen-28-oic acid, T-80126
2,3,6,19-Tetrahydroxy-12-ursen-28-oic acid, T-80127
2,3,7,19-Tetrahydroxy-12-ursen-28-oic acid, T-50183
3,6,19,23-Tetrahydroxy-12-ursen-28-oic acid, T-80129

$C_{30}H_{48}O_7$
3-Acetyl-2-desacetyl-22-epihippurin 1, *in* E-80039
2α-Angeloyloxy-20-(2-methylbutanoyloxy)-8(17),14-labdadiene-3α,7α,13*R*-triol, *in* L-80006
Hippurin 1, *in* E-80039
1α,2α,3β,19α,23-Pentahydroxy-12-ursen-28-oic acid, *in* T-80124

$C_{30}H_{50}$
3,24-Aonenadiene, A-80167
3,4-Di-1-adamantyl-2,2,5,5-tetramethylhexane, D-60025
7,17,21-Podiodatriene, P-80164

$C_{30}H_{50}O$
Achilleol A, A-80032
Cycloeuphordenol, C-70218
Espinenoxide, E-80056
16-Gammaceren-3-ol, G-80003
5-Gluten-3-ol, G-80026
3,7,11,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaen-1-ol, H-80077
24-Isopropenyl-7-cholesten-3-ol, I-70085
13(18)-Lupen-3-ol, L-70043
20(29)-Lupen-7-ol, L-80043
14(26),17,21-Malabaricatrien-3-ol, M-60008
30-Norcyclopterospermol, N-60059
13(18)-Oleanen-3-ol, O-70036
18-Oleanen-3-ol, O-80041
Phyllanthol, P-80141
Pichierenol, P-80145
14-Taraxeren-6-ol, T-80002
4,24,24-Trimethyl-7,25-cholestadien-3-ol, T-80351
19(29)-Ursen-3-ol, U-80034

$C_{30}H_{50}O_2$
23-Cycloartene-3,25-diol, C-80171
24-Cycloartene-1,3-diol, C-80172
20(29)-Epoxy-3-lupanol, E-60026
27-Hydroxy-3-friedelanone, *in* D-70301
24-Isopropenyl-7-cholestene-3,6-diol, I-70084
8,24-Lanostadiene-3,21-diol, L-70017
20(29)-Lupene-3,16-diol, L-60039
20(29)-Lupene-3,16-diol, L-80041
20(29)-Lupene-3,24-diol, L-80042
12-Oleanene-3,15-diol, O-70033
12-Oleanene-3,15-diol, O-80031
12-Oleanene-3,24-diol, O-80032
13(18)-Oleanene-2,3-diol, O-60033
18-Oleanene-3,16-diol, O-80033
α-Onocerol, O-80045
14-Serratene-3,21-diol, S-80027
14-Taraxerene-3,24-diol, T-60008
Trichadenal, T-70218

$C_{30}H_{50}O_3$
5,24-Cucurbitadiene-3,11,26-triol, C-60175
Dihydroniloticin, *in* N-70036
21,27-Dihydroxy-3-friedelanone, D-70301
9(11)-Fernene-3,7,19-triol, F-60002
3α-Hydroxy-27-friedelanoic acid, *in* T-70218
3β-Hydroxy-27-friedelanoic acid, *in* T-70218
3-Hydroxy-28-ursanoic acid, H-80265
8,23-Lanostadiene-3,22,25-triol, L-80019
12-Oleanene-1,3,11-triol, O-60036
12-Oleanene-2,3,11-triol, O-60037
12-Oleanene-2,3,23-triol, O-80037
12-Oleanene-3,15,24-triol, O-80038
12-Oleanene-3,16,28-triol, O-60038
12-Oleanene-3,9,11-triol, O-80039
13(18)-Oleanene-3,16,28-triol, O-70035
13(18)-Oleanene-3,22,24-triol, O-80040
12-Ursene-2,3,11-triol, U-60008

$C_{30}H_{50}O_4$
20,24-Dihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, D-70343
20,25-Dihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, D-70344
7,9(11)-Lanostadiene-3,24,25,26-tetrol, L-60012
11(12)-Oleanene-3,13,23,28-tetrol, O-70034
12-Oleanene-1,2,3,11-tetrol, O-60034
12-Oleanene-3,16,23,28-tetrol, O-60035
12-Oleanene-3,21,22,28-tetrol, O-80036
Quisquagenin, Q-70011
12,20,25-Trihydroxy-23-dammaren-3-one, T-60319
1,11,20-Trihydroxy-3-lupanone, T-60331
3,23,25-Trihydroxy-7-tiracallen-24-one, T-60347
23ξ,24ξ,25-Trihydroxy-7-tirucallen-3-one, *in* P-50204
12-Ursene-1,2,3,11-tetrol, U-60006
12-Ursene-2,3,11,20-tetrol, U-60007

$C_{30}H_{50}O_5$
12-Oleanene-3,16,21,23,28-pentol, O-50037
12-Oleanene-3α,16α,21α,22α,28-pentol, *in* O-80036
12,20,25-Trihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, T-70274
20,25,26-Trihydroxy-3,4-seco-4(28),23-dammaradien-3-oic acid, T-70275
12-Ursene-1,2,3,11,20-pentol, U-60005

$C_{30}H_{50}O_6$
12-Oleanene-3,16,21,22,23,28-hexol, O-80034
Toosendanpentol, T-80202

$C_{30}H_{51}BrO_5$
Magireol *B*, M-60006
Magireol *C*, *in* M-60006

$C_{30}H_{51}BrO_6$
15-Anhydrothyrsiferol, A-60274

$C_{30}H_{52}N_{10}O_7$
Neurotoxin NSTX 3, N-70033

$C_{30}H_{52}O_2$
Espinendiol A, E-80055
3,29-Friedelanediol, F-80082
3,30-Friedelanediol, F-80083
16,22-Hopanediol, H-80096
13,17,21-Polypodatriene-3,8-diol, P-70107

$C_{30}H_{52}O_4$
24-Dammarene-3,6,20,27-tetrol, D-70002
24-Dammarene-3,7,20,27-tetrol, D-70003
Piscidinol B, P-50204
7-Tirucallene-3,23,24,25-tetrol, T-70201

$C_{30}H_{52}O_5$
3,16,24,25,30-Cycloartanepentol, C-60182
24-Dammarene-3,7,18,20,27-pentol, D-70001
25-Dammarene-3,12,17,20,24-pentol, D-60001
1,3,5,6,11-Gorgostanepentol, G-80033

$C_{30}H_{53}BrO_6$
Magireol *A*, M-60005

$C_{30}H_{53}BrO_7$
Thyrsiferol, T-70193
Venustatriol, *in* T-70193

$C_{30}H_{54}$
Hexabutylbenzene, H-60032

$C_{30}H_{58}O_2$
21-Triacontenoic acid, T-80207

$C_{30}H_{60}N_6$
Hexakis(diethylamino)benzene, *in* B-80014

$C_{30}H_{60}O$
Triacontanal, T-80206

$C_{30}H_{60}O_2$
3-Hydroxy-11-triacontanone, H-80257
7-Hydroxy-5-triacontanone, H-80258

$C_{31}H_{18}O$
2,3-Bis(9-anthryl)cyclopropenone, B-70128

$C_{31}H_{20}O_{10}$
Cryptomerin *A*, *in* H-60082
Isocryptomerin, *in* H-60082
Neocryptomerin, *in* H-60082

$C_{31}H_{21}NO_5$
4-Amino-1,7-naphthalenediol; O,O,N-Tribenzoyl, *in* A-80120

$C_{31}H_{22}O_5$
Nordracorubin, N-70075

$C_{31}H_{24}$
4-Methylene-1,2,3,5-tetraphenylbicyclo[3.1.0]hex-2-ene, M-60079

$C_{31}H_{24}O_{12}$
Kolaflavanone, *in* G-70005

$C_{31}H_{27}N_7$
1,14,34,35,36,37,38-Heptaazahepta-cyclo[12.12.7.1^{3,7}.1^{8,12}.1^{16,20}.1^{21,25}.1^{28,32}]octa-triaconta-3,5,7(38),8,10,12(37),16,18,20(36),21,23,25(35),28,30,32(34)penta-decane, H-70010

$C_{31}H_{32}O_8$
Gossypol; 6-Me ether, *in* G-60032

$C_{31}H_{32}O_{12}$
Fridamycin *D*, F-70044

$C_{31}H_{32}O_{16}$
3,4-Di-*O*-caffeoylquinic acid; *O*^{5}-(3-Hydroxy-3-methylglutaroyl), *in* D-70110

$C_{31}H_{36}O_6$
Triptofordin *A*, T-60392

$C_{31}H_{36}O_{18}S$
Rhodonocardin *B*, *in* R-70003

$C_{31}H_{38}O_{10}$
Swietenolide; Di-Ac, *in* S-80054

$C_{31}H_{38}O_{17}$
2′,4′,5,5′,6,7-Hexahydroxyisoflavone; 2′,4′,5′,6-Tetra-Me ether, 7-*O*-rhamnosylglucoside, *in* H-80069

$C_{31}H_{38}O_{18}$
2′,4′,5,5′,6,7-Hexahydroxyisoflavone; 2′,4′,5′,6-Tetra-Me ether, 7-*O*-gentiobioside, *in* H-80069
2′,4′,5,5′,7,8-Hexahydroxyisoflavone; 2′,4′,5′,8-Tetra-Me ether, 7-*O*-gentiobioside, *in* H-80070

$C_{31}H_{39}N_5O_5$
Avellanin *A*, A-60323

$C_{31}H_{40}O_4$
4-*O*-Cadinylangolensin, C-80004

$C_{31}H_{40}O_8$
Khayasin, *in* S-80054

$C_{31}H_{41}NO_6$
Pyrichalasin *H*, P-60215

$C_{31}H_{42}O_6$
6-Deacetoxyhelvolic acid, *in* H-80011

$C_{31}H_{42}O_7$
Helvolinic acid, *in* H-80011

$C_{31}H_{42}O_8$
Fevicordin *A*, F-60008

$C_{31}H_{42}O_{10}$
Ingol; 7-Angeloyl, 3,8,12-tri-Ac, *in* I-70018
Ingol; 7-Tigloyl, 3,8,12-tri-Ac, *in* I-70018
Ingol; 3,7,8-Tri-Ac, 12-tigloyl, *in* I-70018

$C_{31}H_{42}O_{11}$
Euphorianin, E-60074

$C_{31}H_{42}O_{18}$
Radiatoside C, *in* R-80001

$C_{31}H_{42}O_{19}$
Radiatoside B, R-80001

$C_{31}H_{44}O_6$
Anguinomycin *A*, A-70209

$C_{31}H_{44}O_7$
Bufalin; 3-(Me adipoyl), *in* B-70289
Cucurbitacin T, C-80162

$C_{31}H_{46}O_3$
Disidein, D-60499

$C_{31}H_{46}O_7$
Heteronemin; 12-Ac, *in* H-60030
Heteronemin; 12-Epimer, 12-Ac, *in* H-60030

$C_{31}H_{46}O_{13}$
Chamaepitin, C-60033

$C_{31}H_{48}O_3$
3-Oxopisolactone, *in* P-80155

$C_{31}H_{48}O_4$
Regelin, *in* H-70202

$C_{31}H_{48}O_5$
Regelinol, *in* D-70333

$C_{31}H_{50}O$
24-Methylene-7,9(11)-lanostadien-3-ol, M-70072

$C_{31}H_{50}O_2$
δ-Amyrin formate, *in* O-70036
24-Methylene-3,4-seco-4(28)-cycloarten-3-oic acid, M-70078

$C_{31}H_{50}O_3$
Eburicoic acid, E-80001
Pisolactone, P-80155

$C_{31}H_{50}O_4$
2,3-Dihydroxy-12-ursen-28-oic acid; Me ester, *in* D-70349

$C_{31}H_{50}O_5$
7,8-Dihydro-12β-hydroxyholothurinogenin; 12-Me ether, *in* T-70267

$C_{31}H_{50}O_6$
23-Hydroxytormentic acid; Me ester, *in* T-80125

$C_{31}H_{52}O$
Cyclocaducinol, C-80176
Cyclopterospermol, C-60232
3β-Methoxy-18-oleanene, *in* O-80041

$C_{31}H_{52}O_2$
25-Methoxy-23-cycloarten-3β-ol, *in* C-80171
3α-Methoxy-14-serraten-21β-ol, *in* S-80027
3β-Methoxy-14-serraten-21α-ol, *in* S-80027
21β-Methoxy-14-serraten-3β-ol, *in* S-80027
3β-Methoxy-14-serraten-21β-ol, *in* S-80027
24-Methylene-8-lanostene-3,22-diol, M-80087

$C_{31}H_{52}O_3$
22α-Methoxy-13(18)-oleanen-3β,24-diol, *in* O-80040

$C_{31}H_{52}O_6$
21-*O*-Methyltoosendanpentol, *in* T-80202

$C_{31}H_{60}O_2$
12,14-Hentriacontanedione, H-80014
14,16-Hentriacontanedione, H-80015

$C_{31}H_{62}O_2$
Hentriacontanoic acid, H-80016
10-Hydroxy-16-hentriacontanone, H-80170
8-Hydroxy-5-hentriacontanone, H-80171

$C_{32}H_{14}$
Ovalene, O-60046

$C_{32}H_{21}O_{10}$
Muricatin A, *in* D-80345

$C_{32}H_{22}O_{10}$
Chamaecyparin, *in* H-60082
Cryptomerin *B*, *in* H-60082
Floribundone 1, *in* F-80013

$C_{32}H_{24}$
3,6-Bis(diphenylmethylene)-1,4-cyclohexadiene, B-60157

$C_{32}H_{24}N_2O_2$
2,5-Dihydro-3,6-diphenylpyrrolo[3,4-*c*]pyrrole-1,4-dione; 2,5-Dibenzyl, *in* D-70204

$C_{32}H_{24}O_9$
Floribundone 2, F-80013

$C_{32}H_{24}O_{15}$
ε-Isoactinorhodin, I-70059

$C_{32}H_{26}N_2O_9$
5-Vinyluridine; 2′,3′,5′-Tribenzoyl, *in* V-70015

$C_{32}H_{26}N_4O_4$
6,6′-(1,2-Dimethyl-1,2-ethanediyl)bis[1-phenazinecarboxylic acid]; Di-Me ester, *in* D-70411

$C_{32}H_{26}O_8$
2,2′,7,7′-Tetrahydroxy-4,4′8,8′-tetramethoxy-1,1′-biphenanthrene, *in* O-80017

$C_{32}H_{26}O_{13}$
Alterporriol *A*, *in* A-60079
Alterporriol *B*, A-60079
Alterporriol C, A-80054

$C_{32}H_{28}$
5,6,20,21-Tetrahydro-2,16;3,10-diethano-15,11-metheno-11*H*-tribenzo[*a*,*e*,*i*]pentadecene, T-80060

$C_{32}H_{28}O_2$
Dypnopinacol, D-60524

$C_{32}H_{28}O_{10}$
Candicanin, C-80016

$C_{32}H_{30}N_4$
13,15-Ethano-17-ethyl-2,3,12,18-tetramethylmonobenzo[*g*]porphyrin, E-60043

$C_{32}H_{30}O_8$
2′,7-Dihydroxy-4′-methoxy-4-(2′,7-dihydroxy-4′-methoxyisoflavan-5′-yl)isoflavan, D-60347

$C_{32}H_{30}O_9$
Biscyclolobin, B-80145
2′,7-Dihydroxy-4′-methoxy-4-(2′,7-dihydroxy-4′-methoxyisoflavan-5′-yl)isoflavan; 3′-Hydroxy, *in* D-60347

$C_{32}H_{32}O_8$
Toddasin, T-70203

$C_{32}H_{34}N_4O_4$
Corallistin A, C-80150

$C_{32}H_{34}O_7$
Grayanotoxin XIV, *in* G-80039

$C_{32}H_{34}O_8$
Gossypol; 6,6′-Di-Me ether, *in* G-60032

$C_{32}H_{36}O_8$
Artanomaloide, A-60300

$C_{32}H_{36}O_{12}$
Filixic acid ABA, *in* F-80008

$C_{32}H_{38}O_{11}$
6α,11β-Diacetoxygedunin, *in* G-70006

$C_{32}H_{38}O_{15}$
Neoleuropein, N-60018

$C_{32}H_{39}O_{19}^{\oplus}$
Pelagonidin 5-glucoside 3-sambubioside, *in* T-80093

$C_{32}H_{40}O_8$
Hyperevoline, H-70233

$C_{32}H_{40}O_9$
Ingol; O^7-Benzoyl, O^8-Me, 3,12-di-Ac, *in* I-70018

$C_{32}H_{40}O_{10}$
Swietemahonin E, *in* S-80053

$C_{32}H_{40}O_{13}$
Flindercarpin 2, F-80012

$C_{32}H_{40}O_{14}$
Celangulin, *in* H-80027

$C_{32}H_{42}O_8$
Salannic acid; 1-*O*-Tigloyl, Me ester, *in* S-80002

$C_{32}H_{42}O_9$
Trichilinin; 1-Ac, *in* T-60251

$C_{32}H_{44}O_4$
3-Octadecene-1,2-diol; Dibenzoyl, *in* O-60005

$C_{32}H_{44}O_8$
▷ Cucurbitacin *E*, C-70204
Datiscacin, *in* C-70204
Salannol, *in* S-80002

$C_{32}H_{44}O_{13}$
Baccatin I, B-80002

$C_{32}H_{44}O_{14}$
1β-Acetoxy-5-deacetylbaccatin I, *in* B-80002
Baccatin IV, B-80003
1β-Hydroxybaccatin I, *in* B-80002

$C_{32}H_{44}O_{18}$
Isonuezhenide, I-70073

$C_{32}H_{46}O_6$
15α-Acetoxy-3α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70330
3α-Acetoxy-15α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70330
Anguinomycin *B*, A-70210
Azadirachtol, A-70280

$C_{32}H_{46}O_7$
Bufalin; 3-(Hydrogen suberoyl), *in* B-70289
Kasuzamycin *B*, K-70007

$C_{32}H_{48}O_4$
23-Acetoxy-3-oxo-20(30)-lupen-29-al, *in* D-70316
3,4-Seco-4(28),20,24-dammaratrien-3,26-dioic acid; 3-Me ester, *in* S-70021

$C_{32}H_{48}O_5$
15α-Acetoxy-3α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314
3α-Acetoxy-15α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314

$C_{32}H_{48}O_6$
22*S*-Acetoxy-3α,15α-dihydroxy-7,9(11),24-lanostatren-26-oic acid, *in* T-80318
3α-Acetoxy-15α,22*S*-dihydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
22*S*-Acetoxy-3β,15α-dihydroxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318
Chisocheton compound *A*, *in* T-60223

$C_{32}H_{50}O_3$
3β-Acetoxy-21,23-epoxy-7,24-tirucalladiene, *in* E-60032

$C_{32}H_{50}O_4$
23-Acetoxy-30-hydroxy-20(29)-lupen-3-one, *in* D-70318
3β-Acetoxy-28,13β-oleanolide, *in* H-60200
3β-Acetoxy-28,20β-ursanolide, *in* H-60233
Acetylaleuritolic acid, *in* H-80256
Epiacetylaleuritolic acid, *in* H-80256
Niloticin acetate, *in* N-70036

$C_{32}H_{50}O_5$
Alisol *B*; 23-Ac, *in* A-70082
3-Epimesembryanthemoidigenic acid; Ac, *in* D-80347

$C_{32}H_{50}O_6$
21-Acetoxy-21,23:24,25-diepoxyapotirucall-14-ene-3,7-diol, *in* T-60223
16β-Hydroxyalisol B monoacetate, *in* A-70082
Palmitylglutinopallal, *in* G-70021

$C_{32}H_{50}O_7$
Hippurin-2, *in* E-80039

$C_{32}H_{50}O_8$
3-Acetyl-22-epihippurin-1, *in* E-80039
Amphidinolide B, A-70205
Amphidinolide D, *in* A-70205

$C_{32}H_{50}O_{13}$
Medinin, *in* M-70015

$C_{32}H_{52}O_2$
3β-Acetoxy-14(26),17*E*,21-malabaricatriene, *in* M-60008
3β-Acetoxy-19(29)-ursene, *in* U-80034
16-Gammaceren-3-ol; Ac, *in* G-80003
5-Gluten-3-ol; Ac, *in* G-80026
Isopichierenyl acetate, *in* P-80145
Pichierenyl acetate, *in* P-80145

$C_{32}H_{52}O_3$
1α-Acetoxy-24-cycloarten-3β-ol, *in* C-80172
23-Cycloartene-3,25-diol; 3-Ac, *in* C-80171
Eburicoic acid; Me ester, *in* E-80001
Serratenediol 3-monoacetate, *in* S-80027

$C_{32}H_{52}O_4$
22-Acetoxy-8,23-lanostadiene-3α,25-diol, *in* L-80019
3β-Acetoxy-12-oleanene-2α,11α-diol, *in* O-60037
3β-Acetoxy-12-ursene-2α,11α-diol, *in* U-60008
Trichadenal; 27-Carboxylic acid, Ac, *in* T-70218

$C_{32}H_{52}O_5$
3β-Acetoxy-12-oleanene-1β,2α,11α-triol, *in* O-60034
3β-Acetoxy-12-ursene-2α,11α,20β-triol, *in* U-60007
3β-Acetoxy-12-ursene-1β,2α,11α-triol, *in* U-60006

$C_{32}H_{52}O_6$
3β-Acetoxy-12-ursene-1β,2α,11α,20β-tetrol, *in* U-60005

$C_{32}H_{52}O_9$
22-Epitokorogenin; 1-*O*-α-L-Arabinopyranoside, *in* S-60043
Neotokoronin, *in* S-60043
Tokoronin, *in* S-60043

$C_{32}H_{54}$
Meijicoccene, M-70017

$C_{32}H_{54}O_2$
3β,21α-Dimethoxy-14-serratene, *in* S-80027
3β,21β-Dimethoxy-14-serratene, *in* S-80027

$C_{32}H_{54}O_3$
30-Acetoxy-3β-friedelanol, *in* F-80083
3β-Acetoxy-30-friedelanol, *in* F-80083
6-Desoxyleucotylin; 16-Ac, *in* H-80096

$C_{32}H_{54}O_{13}$
ent-2α,16β,17-Kauranetriol; O^2,O^{17}-Bis-β-D-glucopyranoside, *in* K-60004

$C_{32}H_{55}BrO_8$
Thyrsiferol; 23-Ac, *in* T-70193

$C_{32}H_{64}O_4S_2$
1,7,20,26-Tetraoxa-4,23-dithiacyclooctatriacontane, T-80156

$C_{32}H_{64}O_6S_2$
1,7,20,26-Tetraoxa-4,23-dithiacyclooctatriacontane; S,S′-Dioxide, *in* T-80156

$C_{32}H_{64}O_8S_2$
1,7,20,26-Tetraoxa-4,23-dithiacyclooctatriacontane; S,S′-Tetroxide, *in* T-80156

$C_{33}H_{24}O_{13}$
Edgeworoside *A*, E-80007

$C_{33}H_{27}N_7$
Tris[(2,2′-bipyridyl-6-yl)methyl]amine, T-70320

$C_{33}H_{28}O_{10}$
Podocarpusflavanone, P-60163

$C_{33}H_{32}N_4$
13,15-Ethano-3,17-diethyl-2,12,18-trimethylmonobenzo[*g*]porphyrin, E-60042

$C_{33}H_{32}N_4O_2$
13^2,17^3-Cyclopheophorbide enol, C-60230

$C_{33}H_{32}O_9$
2′,7-Dihydroxy-4′-methoxy-4-(2′,7-dihydroxy-4′-methoxyisoflavan-5′-yl)isoflavan; 3′-Hydroxy, 2′-Me ether, *in* D-60347
2′,7-Dihydroxy-4′-methoxy-4-(2′,7-dihydroxy-4′-methoxyisoflavan-5′-yl)isoflavan; 4′-Methoxy, *in* D-60347

$C_{33}H_{36}O_{11}$
Triptofordin *C*-1, *in* T-60394

$C_{33}H_{36}O_{15}$
Pruyanoside A, P-80184

$C_{33}H_{36}O_{16}$
Pruyanoside B, P-80185

$C_{33}H_{38}O_8$
▷ α-Guttiferin, G-60040

$C_{33}H_{38}O_{11}$
9α,14-Diacetoxy-1α,8β-dibenzoyloxy-4β,8β-dihydroxydihydro-β-agarofuran, *in* E-60018
Pringleine, P-60172
Triptofordin *C*-2, T-60394

$C_{33}H_{38}O_{12}$
Filixic acid ABP, *in* F-80008

$C_{33}H_{40}BNO_2$
Muscarine; Tetraphenylborate, *in* M-60153

$C_{33}H_{40}O_{21}$
Isoorientin; 2″,4′-Diglucosyl, *in* I-80068

$C_{33}H_{41}O_{19}$
Pelargonidin 3-(2^{glu}glucosylrutinoside), *in* T-80093

$C_{33}H_{41}O_{19}^{\oplus}$
Pelargonidin 5-glucoside 3-rutinoside, *in* T-80093

$C_{33}H_{41}O_{20}$
Pelargonidin 5-glucoside 3-sophoroside, *in* T-80093

$C_{33}H_{41}O_{20}^{\oplus}$
Orientalin/, *in* T-80093

$C_{33}H_{42}O_4$
Nemorosonol, N-70020

$C_{33}H_{42}O_6$
Vitixanthin, V-80011

$C_{33}H_{42}O_8$
Sarothralen *B*, S-60011

$C_{33}H_{42}O_{19}$
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one; 4′-*O*-Glucopyranosylglucopyranoside, 4″-*O*-glucopyranoside, *in* D-80367

$C_{33}H_{44}O_4$
Eudesobovatol A, E-80088
Eudesobovatol B, E-80089

$C_{33}H_{44}O_6$
Dihydrovitixanthin, *in* V-80011

$C_{33}H_{44}O_8$
▷ Helvolic acid, H-80011

$C_{33}H_{44}O_9$
Volkensin, V-70018

$C_{33}H_{44}O_{16}$
Arctigenin; 4-β-Gentiobioside, *in* A-70249

$C_{33}H_{48}$
3-Methyldotriacontane, M-80072

$C_{33}H_{48}O_{18}$
Macrocliniside *I*, *in* Z-60001

$C_{33}H_{48}O_{19}$
Sylvestroside I, S-70087

$C_{33}H_{52}O_4$
Eburicoic acid; Ac, *in* E-80001

$C_{33}H_{52}O_5$
Saptarangiquinone *A*, S-70009

$C_{33}H_{52}O_6$
22-Acetoxy-3α-hydroxy-7α-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60328
3α-Acetoxy-15α-hydroxy-22-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60327
16β-Methoxyalisol B monoacetate, *in* A-70082

$C_{33}H_{52}O_8$
3-epi-Diosgenin; 3-*O*-β-D-Glucopyranoside, *in* S-60045
Trillin, *in* S-60045

$C_{33}H_{54}O_{12}$
Sileneoside, *in* H-60063

$C_{33}H_{56}O$
23,24,24-Trimethyl-9(11),25-lanostadien-3-ol, T-80352

$C_{33}H_{68}$
2-Methyldotriacontane, M-80071
6-Methyldotriacontene, M-80073
Tritriacontane, T-80369

$C_{34}H_{16}N_4$
29,29,30,30-Tetracyanobianthraquinodimethane, T-60030

$C_{34}H_{18}$
Anthra[9,1,2-*cde*]benzo[*rst*]pentaphene, A-60279
Benzo[*rst*]phenaleno[1,2,3-*de*]pentaphene, B-60036
Benzo[*rst*]phenanthro[10,1,2-*cde*]pentaphene, B-60038
Benzo[*rst*]phenanthro[1,10,9-*cde*]pentaphene, B-60037
Dibenzo[*a,rst*]naphtho[8,1,2-*cde*]pentaphene, D-60075

$C_{34}H_{20}$
5,10-Dihydroanthra[9,1,2-*cde*]benzo[*rst*]pentaphene, *in* A-60279
9,18-Dihydrobenzo[*rst*]phenanthro[10,1,2-*cde*]pentaphene, *in* B-60038

$C_{34}H_{24}O_9$
Mulberrofuran S, M-80195
Plumbazeylanone, P-70106

$C_{34}H_{24}O_{22}$
Pedunculagin, P-80016

$C_{34}H_{26}$
1,3-Bis(1,2-diphenylethenyl)benzene, B-70139

$C_{34}H_{26}O_6$
6,8′-Dihydroxy-2,2′-bis(2-phenylethyl)[5,5′-bi-4*H*-1-benzopyran]-4,4′-dione, D-70289

$C_{34}H_{26}O_{22}$
Cornus-tannin 3, *in* C-80151

$C_{34}H_{30}O_8$
AH_{10}, A-70078

$C_{34}H_{30}O_9$
Semecarpetin, S-70032

$C_{34}H_{34}O_{18}$
Isoorientin; 2″-(4-Hydroxybenzoyl), 4′-β-D-glucopyranoside, *in* I-80068

$C_{34}H_{36}N_4$
13^1-Methyl-13,15-ethano-13^2,17-prop-$13^2(15^2)$-enoporphyrin, M-60082

$C_{34}H_{38}O_{16}$
Cleistanthoside *A*, *in* D-60493

$C_{34}H_{38}O_{17}$
Aloenin *B*, A-60077

$C_{34}H_{40}O_{12}$
Filixic acid ABB, *in* F-80008
Filixic acid PBP, *in* F-80008
Trisabbreviatin BBB, T-60400
Trisaemulin BAB, *in* T-80365

$C_{34}H_{40}O_{16}$
Amorphin, *in* A-80152
Yadanzioside M, Y-80001

$C_{34}H_{42}O_{16}$
Amorphol, *in* A-80152

$C_{34}H_{44}O_9$
Salannin, *in* S-80002

$C_{34}H_{44}O_{10}$
Enukokurin, E-80013

$C_{34}H_{44}O_{13}$
Taccalonolide *B*, T-70001

$C_{34}H_{46}O_{10}S$
Petuniasterone N, P-80074

$C_{34}H_{46}O_{16}$
Bruceantinoside B, B-80269

$C_{34}H_{46}O_{18}$
Loroglossin, L-70037

$C_{34}H_{48}O_7$
3α,15α-Diacetoxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70330

$C_{34}H_{48}O_8$
Ecdysterone 22-*O-benzoate*, *in* H-60063
Pitumbin, P-70104

$C_{34}H_{50}O_6$
Caloverticillic acid *A*, C-60007
Caloverticillic acid *B*, *in* C-60007
Caloverticillic acid *C*, C-60008
3α,15α-Diacetoxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314
3β,15α-Diacetoxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* D-70314

$C_{34}H_{50}O_7$
3α,22ξ-Diacetoxy-15α-hydroxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318
3α,15α-Diacetoxy-22*R*-hydroxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318
3β,15α-Diacetoxy-22*R*-hydroxy-7,9(11)24-lanostatrien-26-oic acid, *in* T-80318
15α,22*S*-Diacetoxy-3α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
3α,22*S*-Diacetoxy-15α-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
15α,22*S*-Diacetoxy-3β-hydroxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318

$C_{34}H_{52}O_5$
3β,23-Diacetoxy-20(30)-lupen-29-al, *in* D-70316

$C_{34}H_{52}O_6$
3β,15α-Diacetoxy-8,24-lanostadien-26-oic acid, *in* D-80331

$C_{34}H_{52}O_7$
3α,7α-Diacetoxy-15α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60327

$C_{34}H_{52}O_8$
3α,22-Diacetoxy-7α,15α-dihydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111

$C_{34}H_{52}O_9$
3,11-Diacetyl-22-epihippurin 1, *in* E-80039
3,11-Diacetylhippurin-1, *in* E-80039
Tiacumicin *A*, T-70194

$C_{34}H_{54}O_4$
18-Oleanene-3,16-diol; Di-Ac, *in* O-80033

$C_{34}H_{54}O_6$
Stearylglutinopallal, *in* G-70021

$C_{34}H_{55}BrO_8$
15(28)-Anhydrothyrsiferyl diacetate, *in* A-60274
15-Anhydrothyrsiferyl diacetate, *in* A-60274

$C_{34}H_{56}O_4$
3β,30-Diacetoxyfriedelane, *in* F-80083

$C_{34}H_{56}O_6$
5,6-Dihydroergosterol; 3-*O*-β-D-Glucopyranoside, *in* M-80059

$C_{34}H_{58}$
Tetramethylsqualene, T-80152

$C_{34}H_{70}O$
1-Tetratriacontanol, T-80161

$C_{35}H_{28}O_{14}$
β-Actinorhodin, A-70062

$C_{35}H_{30}O_{11}$
Kuwanone *L*, K-70016

$C_{35}H_{30}O_{12}$
Hydnowightin, H-70094

$C_{35}H_{36}N_4O_4$
N-Methylprotoporphyrin IX, M-60123

$C_{35}H_{38}O_{11}$
Triptofordin *D*-1, T-60395

$C_{35}H_{38}O_{13}$
Triptofordin *E*, T-60397

$C_{35}H_{40}O_{12}$
Acetylpringleine, *in* P-60172

$C_{35}H_{41}N_5O_6$
Cycloaspeptide *B*, *in* C-70211
Cycloaspeptide *C*, *in* C-70211

$C_{35}H_{42}O_{11}$
1-Cinnamoylmelianone, *in* M-60015

$C_{35}H_{42}O_{12}$
Filixic acid PBB, *in* F-80008

$C_{35}H_{44}O_4$
Neolinderachalcone, *in* N-80021

$C_{35}H_{46}O_4$
Neolinderatin, N-80021

$C_{35}H_{46}O_6$
Mesuaferrol, M-70032

$C_{35}H_{46}O_9$
Trichilinin; 1-*O*-Tigloyl, *in* T-60251

$C_{35}H_{46}O_{19}$
Crassifolioside, C-80155

$C_{35}H_{46}O_{20}$
Echinacoside, E-80004

$C_{35}H_{50}N_8O_6S_2$
Patellamide *A*, P-60011

$C_{35}H_{50}O_{20}$
Sylvestroside II, *in* S-70087

$C_{35}H_{52}O_2$
Plagiospirolide A, P-80156
Plagiospirolide B, P-80157

$C_{35}H_{52}O_{12}$
8,19-Epoxy-17-methyl-1(15)-trinervitene-2,3,7,9,14,17-hexol; 2,3,9,14-Tetrapropanoyl, *in* E-80040
8,19-Epoxy-1(15)-trinervitene-2,3,7,9,14,17-hexol; 2,3,9,14,17-Pentapropanoyl, *in* E-80048

$C_{35}H_{54}O_7$
3α,22-Diacetoxy-7α-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60328

$C_{35}H_{54}O_8$
3α,22-Diacetoxy-15α-hydroxy-7α-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111

$C_{35}H_{56}O_6$
Skimmearepin A, S-80034

$C_{35}H_{56}O_8$
Ilexoside *A*, *in* D-70327
Ilexoside *B*, *in* D-70350

$C_{35}H_{56}O_9$
Cycloorbicoside *A*, *in* C-60218

$C_{35}H_{56}O_{10}$
1,3,19,23-Tetrahydroxy-12-ursen-28-oic acid; *O*-β-D-Xylopyranosyl ester, *in* T-80124

$C_{35}H_{56}O_{11}$
1,3,19,23-Tetrahydroxy-12-ursen-28-oic acid; 2α-Hydroxy, 28-β-D-xylopyranoside, *in* T-80124

$C_{35}H_{58}O_8$
12-Oleanene-3,21,22,28-tetrol; 28-β-D-Xylopyranoside, *in* O-80036

$C_{35}H_{58}O_9$
12-Oleanene-3,21,22,28-tetrol; 16α-Hydroxy, 28-β-D-xylopyranoside, *in* O-80036

$C_{35}H_{61}NO_7$
Pamamycin-607, P-70004

$C_{35}H_{62}O_{12}$
Indicoside *A*, I-60027

$C_{35}H_{63}NO_{12}$
2-Norerythromycin *D*, *in* N-70076

$C_{35}H_{63}NO_{13}$
2-Norerythromycin *C*, *in* N-70076

$C_{35}H_{64}O_7$
Annonacin, A-70212
Goniothalamicin, G-70027

$C_{36}H_{18}O_{16}$
Badione A, B-80007

$C_{36}H_{18}O_{18}$
Badione B, *in* B-80007

$C_{36}H_{22}$
7,16[1′,2′]-Benzeno-7,16-dihydroheptacene, B-70020

$C_{36}H_{24}N_2O_2$
2,2′-(1,4-Phenylene)bis[5,1-[1,1′-biphenyl]-4-yl]oxazole, P-60091

$C_{36}H_{30}O_{14}$
Podoverine *C*, P-60165

$C_{36}H_{30}O_{15}$
Podoverine *B*, *in* P-60165

$C_{36}H_{30}O_{16}$
Salvianolic acid *B*, S-70003

$C_{36}H_{32}O_6$
1,4,7,22,25,28-Hexaoxa[7.7](9,10)anthracenophane, H-70086

$C_{36}H_{32}O_{13}$
Ramosin, R-80002

$C_{36}H_{36}O_8$
α-Diceroptene, D-70112

$C_{36}H_{40}N_2O_{14}S$
Esperamicin *X*, E-70035

$C_{36}H_{43}N_5O_6$
Cycloaspeptide *A*, C-70211

$C_{36}H_{44}O_4$
Panduratin *B*, P-60003

$C_{36}H_{44}O_{12}$
Filixic acid BBB, *in* F-80008
Trisaemulin BBB, *in* T-80365

$C_{36}H_{46}O_{14}$
Taccalonolide *A*, *in* T-70001
Taccalonolide *C*, T-70002
Taccanolide *D*, *in* T-70001

$C_{36}H_{48}O_{18}$
Bruceantinoside *C*, B-70281
Yadanzioside *K*, Y-60001

$C_{36}H_{50}O_8$
β-Ecdysone 2-cinnamate, *in* H-60063

$C_{36}H_{50}O_9$
5β,20*R*-Dihydroxyecdysone; 2-Cinnamoyl, *in* H-60023
β-Ecdysone 3-*p-coumarate*, *in* H-60063

$C_{36}H_{52}O_8$
3β,15α,22*S*-Triacetoxy-7,9(11),24*E*-lanostatrien-26-oic acid, *in* T-80318
3α,15α,22*S*-Triacetoxy-7,9(11),24-lanostatrien-26-oic acid, *in* T-80318

$C_{36}H_{52}O_{12}$
▷ Cucurbitacin *E*; Deacetyl, 2-*O*-β-D-glucopyranosyl, *in* C-70204

$C_{36}H_{52}O_{15}$
Reoselin A, *in* K-80004

$C_{36}H_{54}O_9$
3α,15α,22-Triacetoxy-7α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111
3α,7α,22-Triacetoxy-15α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111
3α,15α,22*S*-Triacetoxy-7α-hydroxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111

$C_{36}H_{54}O_{10}$
Abrusoside *A*, *in* A-80005
Vaccaroside, *in* H-80230

$C_{36}H_{54}O_{12}$
Bryoamaride, *in* C-70204

$C_{36}H_{56}O_{11}$
Ilexsaponin A1, *in* D-60382

$C_{36}H_{58}O_9$
Corchorusin *B*, *in* S-60001
23-Hydroxyimberbic acid; 23-*O*-α-L-Rhamnopyranoside, *in* T-80328

$C_{36}H_{58}O_{10}$
Arjunglucoside II, *in* T-70271
Tormentic acid ester glucoside, *in* T-80342

$C_{36}H_{58}O_{11}$
23-Hydroxytormentic acid ester glucoside, *in* T-80125
7α-Hydroxytormentic acid; 28-*O*-β-D-Glucopyranoside, *in* T-50183
6β-Hydroxytormentic acid; 20-*O*-β-D-Glucopyranoside, *in* T-80127
Hyptatic acid B; 28-*O*-β-D-Glucopyranoside, *in* T-80126
Quercilicoside *A*, *in* T-80125

$C_{36}H_{58}Te_2$
Bis(2,4,6-tri-*tert*-butylphenyl)ditelluride, B-70162

$C_{36}H_{60}O_7$
Inundoside *A*, *in* S-80027
Inundoside E, *in* S-80027

$C_{36}H_{60}O_8$
Corchorusin *A*, *in* O-60038

$C_{36}H_{60}O_9$
Corchorusin *C*, *in* O-60035

$C_{36}H_{62}O_9$
Actinostemmoside *A*, *in* D-70002
Actinostemmoside *B*, *in* D-70003

$C_{36}H_{62}O_{10}$
Actinostemmoside *C*, *in* D-70001

$C_{36}H_{65}NO_{12}$
2-Norerythromycin *B*, *in* N-70076

$C_{36}H_{65}NO_{13}$
2-Norerythromycin, N-70076

$C_{37}H_{42}O_8$
Gambogic acid, G-80002

$C_{37}H_{42}O_{12}$
Triptofordin *D*-2, T-60396

$C_{37}H_{42}O_{14}$
2α,6β,8α,14-Tetraacetoxy-1α,9α-dibenzoyloxy-4β-hydroxydihydro-β-agarofuran, *in* H-80027

$C_{37}H_{46}N_8O_6S_2$
Patellamide *C*, P-60013

$C_{37}H_{46}O_{20}S$
Rhodonocardin *A*, R-70003

$C_{37}H_{46}O_{23}$
Sarothamnoside, *in* T-80309

$C_{37}H_{47}NO_{14}$
▷ Disnogamycin, D-70506

$C_{37}H_{49}N_7O_{12}$
Antibiotic B 1625$FA_{2\beta\text{-}1}$, A-70220

$C_{37}H_{51}BrO_6$
6′-Bromodisidein, *in* D-60499

$C_{37}H_{51}ClO_6$
6′-Chlorodisidein, *in* D-60499

$C_{37}H_{52}O_5$
Aleuritolic acid; 3-(4-Hydroxybenzoyl), *in* H-80256

$C_{37}H_{52}O_{13}$
Fevicordin *A* glucoside, *in* F-60008

$C_{37}H_{53}N_3O_9$
30-Demethoxycurromycin *A*, *in* C-60178

$C_{37}H_{54}O_5$
Oleanderolic acid, *in* T-80344

$C_{37}H_{56}O_9$
23-Hydroxytormentic acid; Me ester, 2,3,23-tri-Ac, *in* T-80125
3α,15α,22*S*-Triacetoxy-7α-methoxy-8,24*E*-lanostadien-26-oic acid, *in* T-60111

$C_{37}H_{56}O_{14}$
Swalpamycin, S-70086

$C_{37}H_{66}O_7$
Bullatacin, B-80273
Bullatacinone, B-80274
4-Hydroxy-25-desoxyneorollinicin, H-80151
Isorollinicin, *in* R-80009
Rollinicin, R-80009

$C_{37}H_{66}O_8$
▷ Bullatalicin, B-80275

$C_{38}H_{18}$
Dibenzo[*jk*,*uv*]dinaphtho[2,1,8,7-*defg*:2′,1′,8′,7′-*opqr*]pentacene, D-60072

$C_{38}H_{26}$
Cycloheptatrienylidene(tetraphenylcyclopentadenylidene)ethylene, C-60208

$C_{38}H_{28}$
[1,1′-Biphenyl]-4,4′-diylbis[diphenylmethyl], B-60117

$C_{38}H_{32}$
5,6,15,16,19,20,29,30-Octahydro-2,17:3,18:7,11:10,14:21,25:24,28-hexamethenobenzocyclooctacosene, O-80014

$C_{38}H_{32}O_2$
2,5-Dimethyl-3,4-diphenyl-2,4-cyclopentadien-1-one; Dimer, *in* D-70403

$C_{38}H_{34}$
5,6,12,13-Tetrahydro-1,17-(ethano[1,3]benzenoethano)-7,11:18,22-dimethenodibenzo[*a*,*h*]cyclooctadecene, T-80062

$C_{38}H_{35}NO_{10}$
Scleroderris green, S-60014

$C_{38}H_{42}O_{12}$
Esulone *A*, E-60038
Esulone *C*, E-60039

$C_{38}H_{42}O_{14}$
Cladochrome, *in* P-70098

$C_{38}H_{46}O_{16}$
Pseudrelone *B*, P-70130

$C_{38}H_{48}N_8O_6S_2$
Patellamide *B*, P-60012

$C_{38}H_{52}O_6$
Pedunculol, P-80017

$C_{38}H_{53}N_3O_{20}S_2$
Antibiotic 273a$_{2\beta}$, *in* A-70218

$C_{38}H_{54}O_{12}$
Datiscoside, *in* C-70203
Datiscoside *B*, *in* C-70203

$C_{38}H_{54}O_{13}$
▷ Elaterinide, *in* C-70204

$C_{38}H_{55}N_3O_{10}$
Curromycin *A*, C-60178

$C_{38}H_{56}O_{11}$
Datiscoside *H*, *in* C-70203

$C_{38}H_{56}O_{13}$
25-*O*-Acetylbryoamaride, *in* C-70204
Datiscoside *G*, *in* C-70203

$C_{38}H_{58}N_4O_8$
Bufalitoxin, *in* B-70289

$C_{38}H_{60}O_{10}$
23-Hydroxyimberbic acid; 1-Ac, 23-*O*-α-L-rhamnopyranoside, *in* T-80328

$C_{38}H_{62}O_8$
Inundoside B, *in* S-80027

$C_{38}H_{64}O_6$
Bacchalatifolin, B-80005

$C_{38}H_{76}O_2$
2-Octadecylicosanoic acid, O-70005

$C_{39}H_{46}O_9$
Trichilinin; 1-*O*-Cinnamoyl, *in* T-60251

$C_{39}H_{48}N_2O_9$
Rubiflavin *F*, R-70012

$C_{39}H_{53}N_9O_{13}S$
Amanullinic acid, *in* A-60084

$C_{39}H_{53}N_9O_{14}S$
▷ Amanine, *in* A-60084
▷ ε-Amanitin, *in* A-60084

$C_{39}H_{53}N_9O_{15}S$
▷ β-Amanitin, *in* A-60084

$C_{39}H_{54}N_{10}O_{12}S$
Amanullin, *in* A-60084

$C_{39}H_{54}N_{10}O_{13}S$
▷ γ-Amanitin, *in* A-60084

$C_{39}H_{54}N_{10}O_{14}S$
▷ α-Amanitin, *in* A-60084

$C_{39}H_{54}O_6$
Isoneriucoumaric acid, *in* D-70349
Neriucoumaric acid, *in* D-70349

$C_{39}H_{55}N_3O_{20}S_2$
Antibiotic 273a$_{2\alpha}$, *in* A-70218

$C_{39}H_{58}O_{15}$
Bryostatin 11, B-70286

$C_{39}H_{62}O_{10}$
▷ Roseofungin, R-70009

$C_{39}H_{62}O_{12}$
Diosgenin; 3-*O*-α-L-Rhamnopyranosyl(1→2)-β-D-glucopyranoside, *in* S-60045
Kallstroemin E, *in* S-60045
Ophiopogonin C′, *in* S-60045

$C_{39}H_{62}O_{13}$
▷ Funkioside *C*, *in* S-60045
Isonuatigenin; 3-*O*-α-L-Rhamnopyranosyl(1→2)-β-D-glucopyranoside, *in* S-60044
Nuatigenin; 3-*O*-α-L-Rhamnopyranosyl(1→2)-β-D-glucopyranoside, *in* N-60062
Trillarin, *in* S-60045

$C_{39}H_{68}O_3$
Defuscin, *in* H-80242

$C_{40}H_{16}$
Phenanthro[3,4,5,6-*bcdef*]ovalene, P-60076

$C_{40}H_{20}$
13,19:14,18-Dimethenoanthra[1,2-*a*]benzo[*o*]pentaphene, D-60396

$C_{40}H_{24}$
Tetrabenzo[*b,h,n,t*]tetraphenylene, T-70012

$C_{40}H_{26}$
9,9′-Bitriptycyl, B-80169

$C_{40}H_{36}O_{10}$
Brosimone *A*, B-70279

$C_{40}H_{36}O_{11}$
Kuwanone *K*, *in* K-70016

$C_{40}H_{38}O_8$
Bianthrone A2b, B-60077
Kuwanon *V*, *in* K-60015

$C_{40}H_{38}O_9$
Kuwanon *Q*, *in* K-60015
Kuwanon *R*, *in* K-60015

$C_{40}H_{38}O_{10}$
Brosimone B, B-80267
Kuwanon *J*, K-60015

$C_{40}H_{40}$
[2.2.2.2.2]Paracyclophane, P-80010

$C_{40}H_{40}O_8$
1,4,7,10,25,28,31,34-Hexaoxa[10.10](9,10)anthracenophane, H-70085

$C_{40}H_{42}N_4O_{17}$
Hydroxymethylbilane, H-70166

$C_{40}H_{42}O_8$
Excelsaoctaphenol, E-80092

$C_{40}H_{42}O_{13}$
Herpetetrone, H-70026

$C_{40}H_{44}O_{13}$
Esulone *B*, *in* E-60038

$C_{40}H_{48}N_6O_9$
RA-II, *in* R-60002
RA-V, R-60002

$C_{40}H_{48}N_6O_{10}$
RA-I, *in* R-60002

$C_{40}H_{48}O_{17}$
Ciclamycin O, C-70176

$C_{40}H_{49}NO_{13}$
Antibiotic TMF 518*D*, A-70240

$C_{40}H_{50}O_{16}$
Ciclamycin 4, *in* C-70176

$C_{40}H_{52}O_3$
Adonirubin, A-70066

$C_{40}H_{52}O_8$
Rosmanoyl carnosate, R-60013

$C_{40}H_{54}O_3$
α-Doradexanthin, D-70545
Fritschiellaxanthin, *in* D-70545

$C_{40}H_{54}O_{10}$
Biperezone; 12,12′-Bis(2-methylbutanoyloxy), *in* B-80105
Biperezone; 12,12′-Bis(3-methylbutanoyloxy), *in* B-80105

$C_{40}H_{56}$
Lycopene, L-60041

$C_{40}H_{56}O$
1,2-Epoxy-1,2-dihydrolycopene, *in* L-60041
5,6-Epoxy-5,6-dihydrolycopene, *in* L-60041

$C_{40}H_{56}O_2$
Rubichrome, R-80014
Tunaxanthin, T-80370

$C_{40}H_{56}O_3$
Eloxanthin, E-80011

$C_{40}H_{56}O_4$
Crustaxanthin, C-80159

$C_{40}H_{56}O_8$
3β,19α-Dihydroxy-24-*trans*-ferulyloxy-12-ursen-28-oic acid, *in* T-60348

$C_{40}H_{58}O_{12}$
Datiscoside *F*, *in* C-70203

$C_{40}H_{58}O_{13}$
Datiscoside *C*, *in* C-70203
Datiscoside *E*, *in* C-70203

$C_{40}H_{60}O_6$
Skimmiarepin B, *in* S-80034

$C_{40}H_{60}O_{13}$
Atratoside *D*, *in* C-70257
Datiscoside *D*, *in* C-70203

$C_{40}H_{66}$
Lycopersene, L-70044

$C_{40}H_{66}O$
15-Hydroxylycopersene, *in* L-70044
2,6,10,14,19,23,27,31-Octamethyl-2,6,10,14,17,22,26,30-dotriacontraoctaen-19-ol, O-70020
Prephytoene alcohol, P-70115

$C_{40}H_{66}O_{12}$
Eryloside A, *in* M-80060

$C_{40}H_{75}NO_9$
1-*O*-β-D-Glucopyranosyl-*N*-(2-hydroxyhexadecanoyl)-4,8-sphingadiene, G-80023

$C_{40}H_{78}$
Lycopadiene, L-60040

$C_{40}H_{78}O$
7,11,15,19-Tetramethyl-3-methylene-2-(3,7,11-trimethyl-2-dodecenyl)-1-eicosanol, T-70138

$C_{41}H_{24}$
Centrohexaindane, C-70031

$C_{41}H_{26}O_{26}$
Alnusiin, A-80048
Vescalagin, V-70006

$C_{41}H_{28}O_{26}$
Liquidambin, L-60029

$C_{41}H_{29}NO$
2,4,6-Triphenyl-*N*-(3,5-diphenyl-4-oxidophenyl)pyridinium betaine, T-80362

$C_{41}H_{30}O_{25}$
Cornus-tannin 2, C-80151

$C_{41}H_{30}O_{26}$
Isoterchebin, I-80092
Terchebin, T-80010

$C_{41}H_{30}O_{27}$
Isorugosin B, I-80088

$C_{41}H_{48}O_{10}$
Nimbolicin, N-80029

$C_{41}H_{50}N_2O_9$
Rubiflavin C_1, R-70011
Rubiflavin C_2, *in* R-70011

$C_{41}H_{50}N_2O_{10}$
Rubiflavin *A*, *in* P-60162

$C_{41}H_{50}N_6O_9$
RA-VII, *in* R-60002

$C_{41}H_{50}N_6O_{10}$
RA-III, *in* R-60002
RA-IV, *in* R-60002

$C_{41}H_{52}N_2O_9$
Rubiflavin *D*, *in* R-70011

$C_{41}H_{52}N_2O_{10}$
Antibiotic SS 21020*C*, A-70238
Rubiflavin *E*, *in* R-70011

$C_{41}H_{52}O_5$
Ferulinolone, F-60006

$C_{41}H_{56}O_3$
(9′*E*)-3′,4′-Didehydro-1′,2′-dihydro-3*R*-hydroxy-1′-methoxy-β,ψ-caroten-19′-al, *in* D-80151

$C_{41}H_{58}O_2$
3′,4′-Didehydro-1′,2′-dihydro-1′-methoxy-β,ψ-caroten-3-ol, D-80151

$C_{41}H_{60}O_{16}$
Neocynaponoside A, *in* N-80019

$C_{41}H_{62}Cl_2O_{12}$
Antibiotic CP 54883, A-70222

$C_{41}H_{62}O_{15}$
Bryostatin 13, B-70288

$C_{41}H_{64}O_{13}$
Gymnemic acid IV, *in* O-80034

$C_{41}H_{66}O_{13}$
Gymnemic acid III, *in* O-80034
Ilexside I, *in* D-70350

$C_{42}H_{18}$
Hexabenzo[*bc,ef,hi,kl,no,qr*]coronene, H-60031

$C_{42}H_{24}$
Tris(9-fluorenylidene)cyclopropane, T-70322

$C_{42}H_{24}S_3$
Tris(thioxanthen-9-ylidene)cyclopropane, T-70326

$C_{42}H_{26}$
9,18-Diphenylphenanthro[9,10-*b*]triphenylene, D-60490

$C_{42}H_{28}$
1,2,3,4-Tetraphenytriphenylene, T-80160

$C_{42}H_{30}$
Hexaphenylbenzene, H-60074

$C_{42}H_{30}N_6O_{12}$
▷ Inositol nicotinate, *in* I-80015

$C_{42}H_{32}O_9$
Canaliculatol, C-70011
Distichol, D-60502
Miyabenol *C*, M-60141

$C_{42}H_{40}O_{14}$
Chokorin, C-70171

$C_{42}H_{44}O_{14}$
8α-Benzoyloxyacetylpringleine, *in* P-60172

$C_{42}H_{46}O_{22}$
Potentillanin, P-80171

$C_{42}H_{46}Si_4$
2,3,9,10-Tetrakis(trimethylsilyl)[5]phenylene, T-60130

$C_{42}H_{62}O_{16}$
Abrusoside *D*, *in* A-80005

$C_{42}H_{64}O_{13}$
Atratoside *A*, *in* A-70267

$C_{42}H_{64}O_{15}$
Abrusoside *C*, *in* A-80005
Bryostatin 10, B-70285
Divaroside, *in* C-70038

$C_{42}H_{64}O_{16}$
Tubocapside *A*, *in* T-70333

$C_{42}H_{68}N_6O_6S$
Dolastatin 10, D-70542

$C_{42}H_{68}O_{13}$
Carnosifloside I, *in* C-60175
Saikosaponin *A*, *in* S-60001

$C_{42}H_{68}O_{16}$
Arjungenin; 3,28-*O*-Bis-β-D-glucopyranosyl, *in* T-70119
23-Hydroxytormentic acid; 3,28-*O*-Bis-β-D-glucopyranosyl, *in* T-80125

$C_{42}H_{72}O_{13}$
Actinostemmoside *D*, *in* D-70002

$C_{42}H_{83}NO_4$
Ergocerebrin, E-80049

$C_{42}H_{84}O_2$
2-Nonacosyl-3-tridecene-1,10-diol, N-70068

$C_{43}H_{48}O_{16}$
Dryocrassin, D-80535

$C_{43}H_{52}N_2O_{11}$
▷ Pluramycin *A*, P-60162

$C_{43}H_{56}O_{17}$
Entandrophragmin, E-70009

$C_{43}H_{58}O_{16}$
Candollein, *in* E-70009

$C_{43}H_{58}O_{17}$
β-Dihydroentandrophragmin, *in* E-70009

$C_{43}H_{62}N_4O_{23}S_3$
Paldimycin *B*, *in* P-70002

$C_{43}H_{64}O_4$
Foliosate, F-80072

$C_{43}H_{64}O_{11}$
Glochidioside N, *in* O-50037

$C_{43}H_{64}O_{16}$
Abrusoside *B*, *in* A-80005

$C_{43}H_{66}O_{14}$
Gymnemic acid I, *in* O-80034

$C_{43}H_{68}O_6$
Corymbivillosol, C-60170

$C_{43}H_{68}O_{12}$
Antibiotic PC 766*B*, A-70228

$C_{43}H_{68}O_{14}$
Gymnemic acid II, *in* O-80034

$C_{44}H_{56}N_8O_7$
Cyclic(*N*-methyl-L-alanyl-L-tyrosyl-D-tryptophyl-L-lysyl-L-valyl-L-phenylalanyl), C-60180

$C_{44}H_{58}O_{12}$
Clibadiolide, C-70187

$C_{44}H_{60}N_4O_{12}$
Halichondramide, H-60003

$C_{44}H_{64}N_4O_{23}S_3$
Paldimycin *A*, *in* P-70002

$C_{44}H_{70}O_{12}$
Antibiotic PC 766*B*′, *in* A-70228

$C_{44}H_{70}O_{16}$
Ophiopogonin D′, *in* S-60045
Polyphyllin *D*, *in* S-60045

$C_{44}H_{72}O_{18}$
Dibenzo-54-crown-18, D-70068

$C_{44}H_{76}O_3$
Thurberin; 3-Tetradecanoyl, *in* L-60039

$C_{44}H_{76}O_{14}$
Portmicin, P-70111

$C_{44}H_{85}NO_{10}$
Acanthocerebroside *C*, A-70009

$C_{44}H_{87}NO_{10}$
Acanthocerebroside *B*, A-70008

$C_{44}H_{90}O$
22-Methyl-22-tritetracontanol, M-80186

$C_{45}H_{44}O_{11}$
Brosimone D, B-80268

$C_{45}H_{46}O_8$
Bianthrone A2a, B-60076

$C_{45}H_{50}O_{19}$
Mangicrocin, M-80005

$C_{45}H_{66}O_9$
Inundoside D_1, *in* S-80027
Inundoside F, *in* S-80027

$C_{45}H_{66}O_{16}$
Bryostatin 2, *in* B-70284

$C_{45}H_{70}O_7$
Corymbivillosol; 3-Ac, *in* C-60170

$C_{45}H_{72}O_{13}$
Oligomycin *E*, O-70039

$C_{45}H_{72}O_{16}$
Dioscin, *in* S-60045
Diosgenin; 3-*O*-[α-L-Rhamnopyranosyl(1→2)][β-D-glucopyranosyl(1→4)-α-L-rhamnopyranosyl(1→4)]-β-D-glucopyranoside, *in* S-60045

$C_{45}H_{72}O_{17}$
Balanitin 3, *in* S-60045
Balanitisin A, *in* S-60045
Deltonin, *in* S-60045
Diosgenin; 3-*O*-β-D-Glucopyranosyl(1→4)-α-L-rhamnopyranosyl(1→4)-β-D-glucopyranoside, *in* S-60045
Diosgenin; 3-*O*-[α-L-Rhamnopyranosyl(1→2)][β-D-glucopyranosyl(1→4)]-β-D-glucopyranoside, *in* S-60045
Gracillin, *in* S-60045
Polypodoside A, P-80167

$C_{45}H_{72}O_{18}$
Diosgenin; 3-*O*-(β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside), *in* S-60045
▷ Funkioside *D*, *in* S-60045

$C_{46}H_{56}MgN_4O_5$
Bacteriochlorophyll f, B-70005

$C_{46}H_{58}O_{27}$
Coptiside *I*, *in* D-70319

$C_{46}H_{66}O_3$
Petroformyne 2, P-80072

$C_{46}H_{68}O_2$
Petroformyne 4, *in* P-80073

$C_{46}H_{68}O_3$
Petroformyne 1, P-80071

$C_{46}H_{70}O_2$
Petroformyne 3, P-80073

$C_{46}H_{72}O_{18}$
Ophiopogonin B′, *in* S-60045

$C_{46}H_{80}O_3$
Thurberin; 3-Hexadecanoyl, *in* L-60039

$C_{46}H_{87}NO_9$
Acanthocerebroside *D*, A-70010

$C_{46}H_{91}NO_{10}$
Acanthocerebroside *A*, A-70007

$C_{47}H_{68}O_{10}$
Inundoside D_2, *in* S-80027

$C_{47}H_{68}O_{17}$
Bryostatin 1, B-70284

$C_{47}H_{76}O_{18}$
Ilexside II, *in* D-70350

$C_{47}H_{80}O_{15}$
▷ Carriomycin, C-60022

$C_{47}H_{80}O_{16}$
Antibiotic W 341*C*, A-70241

$C_{47}H_{89}NO_9$
Acanthocerebroside *E*, A-70011

$C_{48}H_{30}O_{31}$
Castavaloninic acid, *in* V-70006

$C_{48}H_{32}O_{30}$
Bicornin, B-80073

$C_{48}H_{36}$
[2_6]Paracyclophene, P-70009
7,10:19,22:31,34-Triethenotribenzo[*a,k,u*]cyclotriacontane, T-60273

$C_{48}H_{36}O_{12}$
1,2,3,4,5,6-Hexa-*O*-benzoyl-*myo*-inositol, *in* I-80015

$C_{48}H_{54}O_{27}$
Safflor Yellow B, S-70001

$C_{48}H_{64}Br_2N_4$
Octaethyltetramethyl[26]porphyrin[3.3.3.3]; Dibromide, *in* O-60008

$C_{48}H_{64}N_4^{2\oplus}$
Octaethyltetramethyl[26]porphyrin[3.3.3.3], O-60008

$C_{48}H_{72}O_3$
5-Methoxy-2-methyl-3-octaprenyl-1,4-benzoquinone, *in* M-80046

$C_{48}H_{72}O_{15}$
Glochidioside, *in* O-50037

$C_{48}H_{72}O_{18}$
Atratoside *C*, *in* A-70267

$C_{48}H_{74}O_{18}$
Atratoside *B*, *in* A-70267

$C_{48}H_{74}O_{19}$
Chiisanoside, *in* C-70038

$C_{48}H_{74}O_{21}$
Tubocapside *B*, *in* T-70333

$C_{48}H_{76}O_{19}$
Saponin *A*, *in* C-70002

$C_{48}H_{77}N_7O_{16}$
Mulundocandin, M-70157

$C_{48}H_{78}O_{18}$
Carnosifloside II, *in* C-60175
Carnosifloside III, *in* C-60175
Carnosifloside IV, *in* C-60175

$C_{48}H_{78}O_{19}$
▷ Asiaticoside, *in* T-80343

$C_{48}H_{80}O_{18}$
Carnosifloside V, *in* C-60175
Carnosifloside VI, *in* C-60175

$C_{48}H_{91}NO_9$
Acanthocerebroside *F*, A-70012

$C_{49}H_{66}O_{28}$
Oleonuezhenide, O-70037

$C_{49}H_{72}O_{17}$
Bryostatin 12, B-70287

$C_{49}H_{74}O_{16}$
Glochidioside Q, *in* O-50037

$C_{49}H_{75}N_7O_{15}$
Antibiotic FR 900359, A-70223

$C_{49}H_{75}N_{13}O_{12}$
Cyanoviridin *RR*, C-70210

$C_{50}H_{44}O_{10}$
Disain, D-80517

$C_{50}H_{58}O_{18}$
Cerberalignan H, C-80036

$C_{50}H_{63}BrO_{16}$
Bromothricin, *in* C-60137

$C_{50}H_{63}ClO_{16}$
Chlorothricin, C-60137

$C_{50}H_{63}ClO_{17}$
2‴-Hydroxychlorothricin, *in* C-60137

$C_{50}H_{80}O_{21}$
Balanitin 2, *in* S-60045
Pariphyllin B, *in* S-60045

$C_{50}H_{80}O_{22}$
▷ Funkioside *F*, *in* S-60045
Saponoside A, *in* S-60045

$C_{51}H_{72}Cl_2O_{18}$
Lipiarmycin A_4, *in* L-60028
Tiacumicin *E*, T-70197

$C_{51}H_{76}O_2$
2-[3,7,11,15,19,23-Hexamethyl-25-(2,6,6-trimethyl-2-cyclohexenyl)pentacosa-2,14,18,22-tetraenyl]-3-methyl-1,4-naphthoquinone, H-70084

$C_{51}H_{80}O_{20}$
Deltofolin, *in* S-60045

$C_{51}H_{82}O_{20}$
Kallstroemin D, *in* S-60045

$C_{51}H_{82}O_{21}$
Pariphyllin A, *in* S-60045

$C_{51}H_{82}O_{22}$
Aculeatiside *A*, *in* N-60062
Balanitin 1, *in* S-60045
Funkioside *E*, *in* S-60045
Kikubasaponin, *in* S-60045

$C_{51}H_{82}O_{23}$
Aculeatiside *B*, *in* N-60062
Avenacoside *A*, *in* N-60062

$C_{51}H_{102}O$
26-Henpentacontanone, H-70009

$C_{52}H_{30}N_4$
37*H*,39*H*-Tetranaphtho-[2,3-*b*:2′,3′-*g*:2″,3″-*l*:2‴-3‴-*q*]porphine, T-80155

$C_{52}H_{74}Cl_2O_{18}$
Lipiarmycin A_3, *in* L-60028
Tiacumicin *C*, T-70195
Tiacumicin *D*, T-70196
Tiacumicin *F*, T-70198

$C_{52}H_{82}O_{20}$
Guaianin *D*, *in* H-60199

$C_{53}H_{31}N_3$
2,12-Di-9-acridinyl-7-phenyldibenz[*c*,*h*]acridine, D-70033

$C_{53}H_{80}O_3$
5-Methoxy-2-methyl-3-nonaprenyl-1,4-benzoquinone, *in* M-80046

$C_{53}H_{84}O_{24}$
Camellidin II, *in* D-60363

$C_{54}H_{90}O_{22}$
Verbascosaponin, *in* O-70034

$C_{55}H_{32}O_{34}$
Daviciin M_1, D-80005

$C_{55}H_{74}IN_3O_{21}S_4$
Calichemicin γ_1^I, C-70008

$C_{55}H_{78}O_2$
2-(3,7,11,15,19,23,27,31,35-Nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonenyl)-1,4-benzoquinone, N-80070

$C_{55}H_{82}O_{21}S_2$
▷ Yessotoxin, Y-60002

$C_{55}H_{84}N_{16}O_{20}$
Pyoverdin II, P-70149

$C_{55}H_{85}N_{17}O_{19}$
Pyoverdin III, *in* P-70149

$C_{55}H_{85}N_{17}O_{22}$
Pyoverdin *D*, P-70147

$C_{55}H_{86}N_{18}O_{21}$
Pyoverdin *E*, *in* P-70147

$C_{55}H_{86}O_{25}$
Camellidin I, *in* D-60363

$C_{56}H_{40}$
Tetrakis(diphenylmethylene)cyclobutane, T-70128

$C_{56}H_{40}O_{12}$
Miyabenol *B*, M-60140

$C_{56}H_{42}O_{12}$
Miyabenol *A*, M-60139
Vaticaffinol, V-60002

$C_{56}H_{44}O_{13}$
Kobophenol A, K-80011

$C_{56}H_{52}N_4Zn$
5,10,15,20-Tetrakis(2,4,6-trimethylphenyl)-21*H*,23*H*-porphine; Zn complex, *in* T-80134

$C_{56}H_{54}N_4$
5,10,15,20-Tetrakis(2,4,6-trimethylphenyl)-21*H*,23*H*-porphine, T-80134

$C_{56}H_{84}N_{16}O_{21}$
Pyoverdin I, P-70148

$C_{56}H_{85}N_{17}O_{23}$
Pyoverdin *C*, P-70146

$C_{57}H_{86}O_3$
2-Decaprenyl-6-methoxy-1,4-benzoquinone, D-80013

$C_{57}H_{92}O_{28}$
Avenacoside *B*, *in* N-60062

$C_{58}H_{78}N_4O_{22}S_4$
Esperamicin A_{1b}, *in* E-60037

$C_{58}H_{88}O_3$
3- Decaprenyl-5-methoxy-2-methyl-1,4-benzoquinone, *in* M-80046

$C_{58}H_{92}O_{52}$
Guaianin *E*, *in* H-60199

$C_{59}H_{80}N_4O_{22}S_4$
Esperamicin A_1, *in* E-60037
Esperamicin A_2, *in* E-60037

$C_{59}H_{90}O_{26}$
▷ Funkioside *G*, *in* S-60045

$C_{60}H_{48}O_{15}$
Lophirochalcone, L-80036

$C_{60}H_{68}O_{21}$
Cerberalignan I, C-80037

$C_{60}H_{78}O_9$
Rzedowskia bistriterpene, R-80018
Rzedowskia bistriterpene; 4-Epimer, *in* R-80018

$C_{62}H_{36}O_2$
9,11,20,22-Tetraphenyltetrabenzo[*a*,*c*,*l*,*n*]pentacene-10,21-dione, T-70151

$C_{62}H_{38}$
b,*b*′,*b*″-Tritriptycene, T-60407

$C_{62}H_{40}N_6O_2P_2$
2,4,5-Tris(dicyanomethylene)-1,3-cyclopentanedione; Bis(tetraphenylphosphonium salt), *in* T-70321

$C_{63}H_{98}N_{18}O_{13}S$
Substance *P*, S-60059

$C_{68}H_{130}N_2O_{23}P_2$
Lipid *A*, L-70032

$C_{70}H_{68}$
1,3,5,7-Tetrakis[2-D_3-trishomocubanyl-1,3-butadiynyl]adamantane, T-70129

$C_{73}H_{108}N_{16}O_{18}S$
Rhodotorucin *A*, R-70004

$C_{73}H_{126}O_{20}$
Bistheonellide *B*, *in* M-60138

$C_{74}H_{73}O_{37}^{\oplus}$
Zebrinin, Z-70002

$C_{74}H_{128}O_{20}$
Misakinolide *A*, M-60138

$C_{75}H_{118}O_{40}$
Vacsegoside, *in* H-80230

$C_{76}H_{124}O_{33}$
Capsianside A, C-80018

$C_{79}H_{91}O_{45}^{\oplus}$
Heavenly blue anthocyanin, H-70006

$C_{80}H_{126}O_{44}$
Gypsoside, *in* H-80230

$C_{81}H_{84}Cl_2N_8O_{29}$
Parvodicin *A*, *in* P-70012

$C_{82}H_{52}$
Tetra(2-triptycyl)ethylene, T-60169

$C_{82}H_{86}Cl_2N_8O_{29}$
Antibiotic A 40926*A*, *in* A-70219
Parvodicin B_1, *in* P-70012
Parvodicin B_2, *in* P-70012

$C_{83}H_{88}Cl_2N_8O_{29}$
Antibiotic A 40926*B*, *in* A-70219
Parvodicin C_1, *in* P-70012
Parvodicin C_2, *in* P-70012

$C_{85}H_{90}Cl_2N_8O_{30}$
Parvodicin C_3, *in* P-70012
Parvodicin C_4, *in* P-70012

$C_{98}H_{141}N_{25}O_{23}S_4$
Epidermin, E-70010

$C_{100}H_{164}O$
Dolichol, D-60517

$C_{102}H_{78}S_6$
6*H*,24*H*,26*H*,38*H*,56*H*,58*H*-16,65:48,66-Bis([1,3]benzenomethanothiomethano[1,3]benzeno)-32,64-etheno-1,5:9,13:14,18:19,-23:27,31:33,37:41,45:46,50:51,55:59,63-decemetheno-8*H*,40*H*[1,7]dithiacyclotetratriacontino[9,8-*h*][1,77]dithiocyclotetratriacontin, B-70129

$C_{104}H_{104}N_8O_{14}$
7,8,9,10,24,25,27,28,30,31,33.34,36,37,39,40,54,55,56,57,71,72,74,75,77,78,80,1,83,84,86,87-Dotriacontahydro-1,93:4,6:11,13:16,18:19,22:42,45:46,48:51,53:58,60:63,65:66,69:89,92-dodecathenotetrabenzo[z_1j_1,q_2,a_3][1,4,7,10,13,16,19,44,47.50,53,56,59,62,25,28,35,38,68,71,78,81]tetradecaoxaotaazacyclohexaoctacontine, D-80529

$C_{122}H_{210}N_2O_{16}$
[3][14-Acetyl-14-azacyclohexacosanone][25,26,53,54,55,56-hexaacetoxytricyclo[49.3.1.1^{24,28}]hexapentaconta-1(55),24,26,28(56),51,53-hexaene][14-acetyl-14-azacyclohexacosanone]catenane, A-60020

$C_{250}H_{410}N_{68}O_{75}$
Thymopoietin I, *in* T-70192

$C_{251}H_{412}N_{64}O_{78}$
Thymopoietin II, *in* T-70192

$C_{255}H_{416}N_{66}O_{77}$
Thymopoietin III, *in* T-70192